

10/751,824

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alerts (SDIs) affected
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NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN
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NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and
February 2005
NEWS 17 JAN 26 CA/CAPLUS - Expanded patent coverage to include the Russian
Agency for Patents and Trademarks (ROSPATENT)

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability
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=> fil casreact
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FILE CONTENT:1840 - 23 Jan 2005 VOL 142 ISS 4

*
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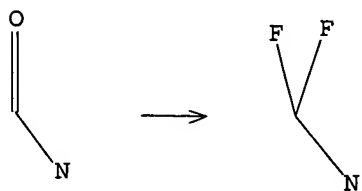
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chain nodes :
1 2 3 4 5 6 7 8
chain bonds :
1-2 2-3 4-5 4-6 5-7 5-8
exact/norm bonds :
1-2 2-3 4-5 5-7 5-8
exact bonds :
4-6

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS
fragments assigned product role:
containing 4
fragments assigned reactant/reagent role:
containing 1

L1	STR
----	-----



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 15:50:41 FILE 'CASREACT'

SCREENING COMPLETE - 5 REACTIONS TO VERIFY FROM 3 DOCUMENTS

100.0% DONE 5 VERIFIED 2 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 5 TO 234

PROJECTED ANSWERS: 1 TO 79

```
L2          1 SEA SSS SAM L1 (      2 REACTIONS)
```

=> s ll full

FULL SEARCH INITIATED 15:50:46 FILE 'CASREACT'

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100.0% DONE 395 VERIFIED 136 HIT RXNS 47 DOCS

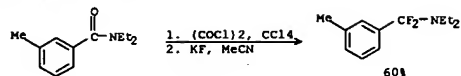
SEARCH TIME: 00.00.01

L3 47 SEA SSS FUL L1 (136 REACTIONS)

=> d 13 1-47

L3 ANSWER 1 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

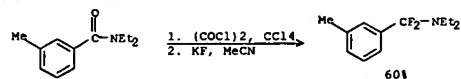
RX(41) OF 51 - 2 STEPS



REF: PCT Int. Appl., 2004050676, 17 Jun 2004

L3 ANSWER 2 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

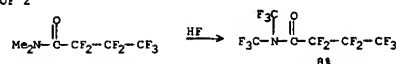
RX(9) OF 9 - 2 STEPS



REF: Jpn. Kokai Tokkyo Koho, 2003064034, 05 Mar 2003

L3 ANSWER 3 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

RX(2) OF 2

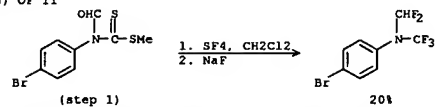


REF: Proceedings - Electrochemical Society, 2001-14(Reactive Intermediates in Organic and Biological Electrochemistry), 113-116; 2001

NOTE: Electrochem.

L3 ANSWER 4 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

RX(8) OF 11

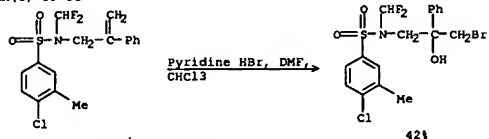


REF: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii), 36(8), 1173-1177; 2000

NOTE: thermal

L3 ANSWER 5 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

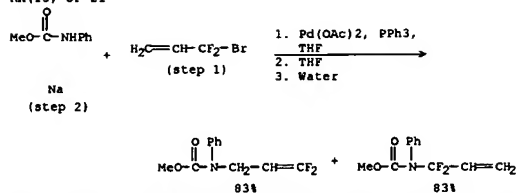
RX(6) OF 11



REF: Nippon Noyaku Gakkaishi, 26(1), 1-8; 2001

L3 ANSWER 6 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

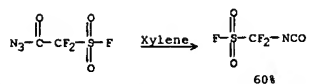
RX(13) OF 21



REF: Chemical & Pharmaceutical Bulletin, 48(6), 885-888; 2000
NOTE: stereoselective, regioselective

L3 ANSWER 7 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

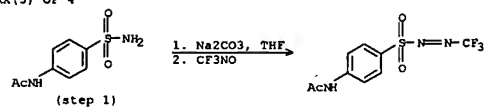
RX(9) OF 21



REF: Journal of Fluorine Chemistry, 84(2), 135-139; 1997
NOTE: thermal

L3 ANSWER 8 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

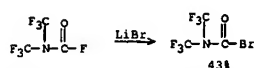
RX(3) OF 4



REF: Zeitschrift fuer Naturforschung, B: Chemical Sciences, 52(5), 647-654; 1997
NOTE: NO YIELD GIVEN

L3 ANSWER 9 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

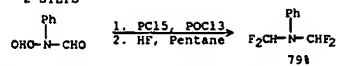
RX(6) OF 10



REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry, (9), 915-920; 1996

L3 ANSWER 10 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

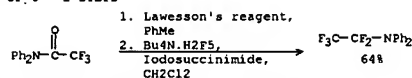
RX(3) OF 3 - 2 STEPS



REF: Journal of Fluorine Chemistry, 76(1), 95-8; 1996

L3 ANSWER 11 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

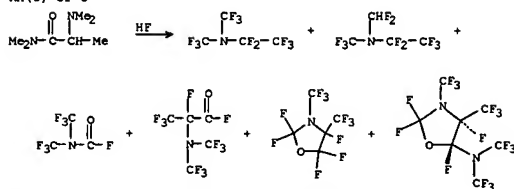
RX(5) OF 6 - 2 STEPS



REF: Tetrahedron Letters, 35(23), 3983-4; 1994

L3 ANSWER 12 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

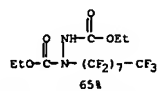
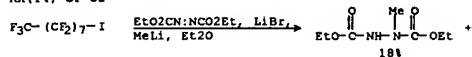
RX(3) OF 3



REF: Journal of Fluorine Chemistry, 48(2), 257-79; 1990
NOTE: electrochem.

L3 ANSWER 13 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

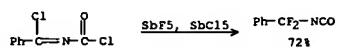
RX(14) OF 32



REF: Bulletin of the Chemical Society of Japan, 62(8), 2636-42; 1989

L3 ANSWER 14 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

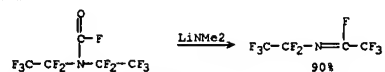
RX(2) OF 5



REF: Zhurnal Organicheskoi Khimii, 25(7), 1572-3; 1989

L3 ANSWER 15 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

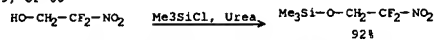
RX(2) OF 26



REF: Journal of Fluorine Chemistry, 45(2), 293-311; 1989

L3 ANSWER 16 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

RX(29) OF 68



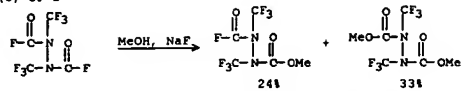
REF: Zhurnal Obshchei Khimii, 58(10), 2274-81; 1988

RX(11) OF 15



REF: Khimiko-Farmatsevticheskii Zhurnal, 22(11), 1339-43; 1988

RX(3) OF 3



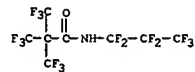
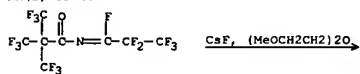
REF: Journal of Fluorine Chemistry, 34(2), 251-4; 1986

RX(1) OF 13



REF: Zeitschrift fuer Anorganische und Allgemeine Chemie, 537,, 63-78; 1986

RX(2) OF 48

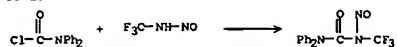


Cs

REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (11), 2533-7; 1985

L3 ANSWER 21 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

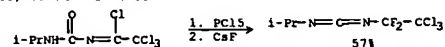
RX(13) OF 29



REF: Nippon Kagaku Kaishi, (11), 2205-7; 1985

L3 ANSWER 22 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

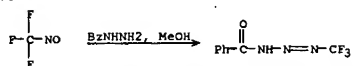
RX(33) OF 54 - 2 STEPS



REF: Zhurnal Organicheskoi Khimii, 20(12), 2543-8; 1984

L3 ANSWER 23 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

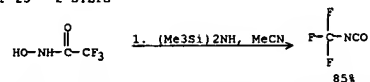
RX(6) OF 11



REF: Bulletin of the Chemical Society of Japan, 57(10), 2962-4; 1984

L3 ANSWER 24 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

RX(16) OF 23 - 2 STEPS



REF: Journal of Organic Chemistry, 49(23), 4541-3; 1984

L3 ANSWER 25 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

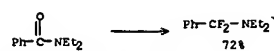
RX(4) OF 5



REF: Zhurnal Obshchei Khimii, 54(2), 477-8; 1984

L3 ANSWER 26 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

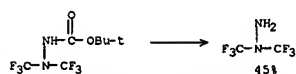
RX(1) OF 12



REF: Polish Journal of Chemistry, 56(10-12), 1369-78; 1982

L3 ANSWER 27 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

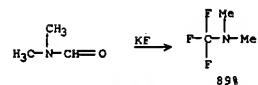
RX(3) OF 11



REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (2), 436-8; 1984

L3 ANSWER 28 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

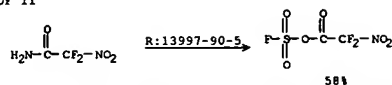
RX(2) OF 13



REF: Journal of Fluorine Chemistry, 23(3), 207-18; 1983

L3 ANSWER 29 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

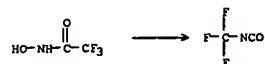
RX(9) OF 11



REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (9), 2134-6; 1983

L3 ANSWER 30 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

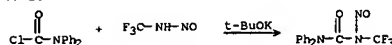
RX(25) OF 39 - 2 STEPS



REF: Journal of Organic Chemistry, 48(21), 3845-7; 1983

L3 ANSWER 31 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

RX(13) OF 28



REF: Journal of Fluorine Chemistry, 22(1), 91-4; 1983

L3 ANSWER 32 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

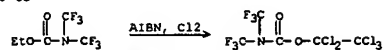
RX(2) OF 10



REF: Journal of Fluorine Chemistry, 21(3), 329-34; 1982

L3 ANSWER 33 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

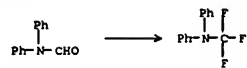
RX(1) OF 12



REF: Zhurnal Organicheskoi Khimii, 18(10), 2220-1; 1982

L3 ANSWER 34 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

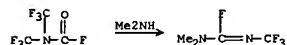
RX(4) OF 6 - 2 STEPS



REF: Ger. Offen., 3044216, 16 Jun 1982

L3 ANSWER 35 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

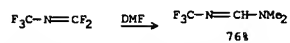
RX(15) OF 34



REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (11), 2632-5; 1981

L3 ANSWER 36 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

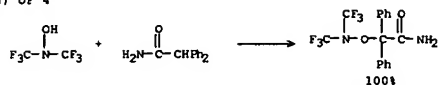
RX(1) OF 3



REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (9), 2168; 1981

L3 ANSWER 37 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

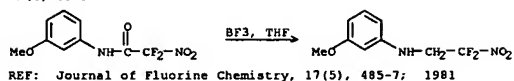
RX(4) OF 4



REF: Journal of Fluorine Chemistry, 17(6), 561-4; 1981

L3 ANSWER 38 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

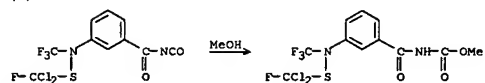
RX(1) OF 9



REF: Journal of Fluorine Chemistry, 17(5), 485-7; 1981

L3 ANSWER 39 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

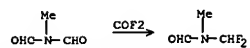
RX(1) OF 1



REF: Ger. Offen., 2938111, 16 Apr 1981

L3 ANSWER 40 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

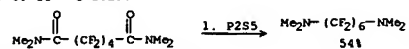
RX(1) OF 5



REF: Zeitschrift fuer Anorganische und Allgemeine Chemie, 474,, 7-17; 1981

L3 ANSWER 41 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

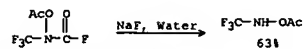
RX(10) OF 11 - 2 STEPS



REF: Zhurnal Organicheskoi Khimii, 16(12), 2508-13; 1980

L3 ANSWER 42 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

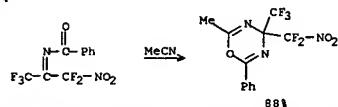
RX(1) OF 8



REF: Journal of Fluorine Chemistry, 15(3), 183-9; 1980

L3 ANSWER 43 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

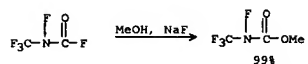
RX(5) OF 24



REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (8), 1826-30; 1979

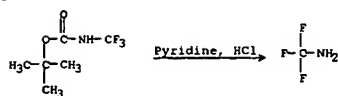
L3 ANSWER 44 OF 47 CASREACT COPYRIGHT 2005 ACS on STN

RX(11) OF 16



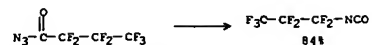
REF: Journal of Fluorine Chemistry, 14(4), 289-97; 1979

RX(4) OF 22



REF: Chemische Berichte, 112(6), 2158-66; 1979

RX(2) OF 3

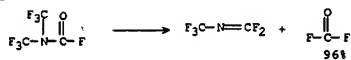


REF: Monatshefte fuer Chemie, 95(2), 608-16; 1964

NOTE: Classification: Rearrangement; Nitrene Intermediate; #

Conditions: -70 deg to Rf; # Comments: yield >84%

RX(1) OF 1



REF: Journal of the American Chemical Society, 78,, 5637-9; 1956

NOTE: Classification: Thermolysis; Elimination; # Conditions: /N2 /P

575 deg

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

232.45

232.66

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DICTIONARY FILE UPDATES: 27 JAN 2005 HIGHEST RN 821767-00-4

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Experimental and calculated property data are now available. For more
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=> s (oxalyl fluoride)/cn

L4 1 (OXALYL FLUORIDE)/CN

=> d l4

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 359-40-0 REGISTRY
 CN Ethanedioyl difluoride (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Oxalyl fluoride (6CI, 7CI, 8CI)
 OTHER NAMES:
 CN Oxalyl difluoride
 FS 3D CONCORD
 MF C2 F2 O2
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPIUS, CASREACT, CHEMCATS,
 CHEMINFORMRX, CHEMLIST, CSCHM, DETHERM*, GELIN*, MSDS-OHS, RTECS*,
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 DT.CA Capius document type: Dissertation; Journal; Patent; Report
 RL.P Roles from patents: PREP (Preparation); PROC (Process); RACT (Reactant
 or reagent); USES (Uses)
 RLD.P Roles for non-specific derivatives from patents: PREP (Preparation)
 RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation,
 nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process);
 PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No
 role
 in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

155 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 155 REFERENCES IN FILE CAPIUS (1907 TO DATE)
 6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> s difluorophosgene/cn
L5      1 DIFLUOROPHOSGENE/CN

=> d 15
```

RN 353-50-4 REGISTRY
 CN Carbonic difluoride (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Carbonyl fluoride (6CI, 8CI)
 OTHER NAMES:
 CN Carbon difluoride oxide
 CN Carbon fluoride oxide (COF2)
 CN Carbon oxyfluoride
 CN Carbon oxyfluoride (COF2)
 CN Carbonyl difluoride
 CN Carbonyl difluoride (COF2)
 CN Carbonyl fluoride
 CN Difluoroformaldehyde
 CN Difluorooxomethane
 CN Difluorophosgene
 CN Fluoroformyl fluoride
 CN Fluorophosgene
 FS 3D CONCORD
 MF C F2 O
 CI COM
 LC STN Files: ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CBMB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCEM, CSMB, DETHERM*, DIPPR*, GHELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDS, MRCK*, MSDS-OHS, NIOSHTIC, PROMT, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**, NDSL**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)
 DT.CA CAplus document type: Conference; Dissertation; Journal; Patent;
 Report
 RL.P Roles from patents: ANST (Analytical study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
 RLD.P Roles for non-specific derivatives from patents: PREP (Preparation)
 RLD.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
 RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1255 REFERENCES IN FILE CA (1907 TO DATE)
 5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1255 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 126 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his

(FILE 'HOME' ENTERED AT 15:50:09 ON 28 JAN 2005)

FILE 'CASREACT' ENTERED AT 15:50:21 ON 28 JAN 2005

L1 STRUCTURE UPLOADED
L2 1 S L1
L3 47 S L1 FULL

FILE 'REGISTRY' ENTERED AT 15:51:29 ON 28 JAN 2005

L4 1 S (OXALYL FLUORIDE)/CN
L5 1 S DIFLUOROPHOSGENE/CN

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

14.60

247.26

FILE 'CAPLUS' ENTERED AT 15:53:45 ON 28 JAN 2005

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FILE COVERS 1907 - 28 Jan 2005 VOL 142 ISS 6

FILE LAST UPDATED: 27 Jan 2005 (20050127/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L6 47 L3

=> s 353-50-4/rn

1255 353-50-4

5 353-50-4D

L7 1252 353-50-4/RN

(353-50-4 (NOTL) 353-50-4D)

=> s l6 and l7

L8 4 L6 AND L7

=> s 359-40-0/rn

155 359-40-0

1 359-40-0D

L9 154 359-40-0/RN

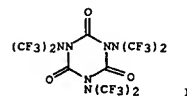
(359-40-0 (NOTL) 359-40-0D)

=> s 16 and 19
L10 0 L6 AND L9

=> d 18 1-4 abs ibib

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Tetramethylammonium salts, Me₃N+CHF₂ (I), Me₃N+CHF₂ (II), and Me₃N+CF₃ (III), were prepared by quaternization of the corresponding fluoromethylamines. II was also generated from Me₃N and Zn-CF₂Br₂-KF in MeCN. I, II, and III were characterized by NMR and vibrational spectroscopy, a normal coordinate anal. being undertaken for III. The crystal structures of the iodides of II and III have been determined. In both cations the N-Me distances are on the average (II 1.508(2) Å; III 1.514(5) Å) longer than the N-CF valencies (II 1.497(4) Å; III 1.491(6) Å).
 ACCESSION NUMBER: 1987:477261 CAPLUS
 DOCUMENT NUMBER: 107:77261
 TITLE: Synthesis, vibrational spectra, and crystal structure analysis of di- and trifluoro-tetramethylammonium salts
 AUTHOR(S): Brauer, D. J.; Buerger, H.; Grunwald, M.; Pawelke, Wilke, J.
 G.: Anorg. Chem., Univ. Gesamthochsch., Wuppertal, Fed. Rep. Ger.
 CORPORATE SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (1986), 537, 63-78
 SOURCE: CODEN: ZAACAB; ISSN: 0044-2313
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 107:77261

L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 GI



AB (CF₃)₂NCOF (I) reacted with P(OR)₃ (R = Me, Et) to give F₂P(OR)₃ and CF₃N:CFPF(OR)₃, with R₂NH (R = Me, Et) to give CF₃C:CFN₂, and with NaN₃ to give I. The reaction mechanisms involved displacement of (CF₃)₂N- from I by the nucleophile to form a fluorocarbonyl derivative of the nucleophile and CF₃N:CF₂ and further reactions of these species.
 ACCESSION NUMBER: 1982:51430 CAPLUS
 DOCUMENT NUMBER: 96:51430
 TITLE: Reactions of bis(trifluoromethyl)carbamoyl fluoride with nucleophilic reagents
 AUTHOR(S): Gontar, A. F.; Bykhovskaya, E. G.; Vinogradov, A. S.; Knunyants, I. L.
 CORPORATE SOURCE: Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR
 SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1981), (11), 2632-5
 CODEN: IASKA6; ISSN: 0002-3353
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 96:51430

L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Fluorinating RN(CHC12)2 (R = Me, Et) and N(CHC12)3 with SbF₃ gave RN(CHF₂)2 and N(CHF₂)3, resp. Under certain conditions, MeN(CHO)2 with COF₂ gave the known MeN(CHO)CHF₂. RN(CHF₂)2 and N(CHF₂)3 are mols. with covalent C-F bonds. Treating MeN(CHF₂)2 with SbF₅ or BF₃ cleaved a F- ion from a CHF₂ group to give [MeN(CHF₂)2:CHF]+ X- (X = SbF₆ or BF₄).
 ACCESSION NUMBER: 1981:442254 CAPLUS
 DOCUMENT NUMBER: 95:42254
 TITLE: Preparation and study of difluoromethyl-substituted amines
 AUTHOR(S): Allenstein, E.; Schrempf, G.
 CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
 SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (1981), 474, 7-17
 CODEN: ZAACAB; ISSN: 0044-2313
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 95:42254

L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 GI For diagram(s), see printed CA Issue.
 AB Me₂NCOCl (I) (1423 g.) in anhydrous HF (3.5 mole-% initial concentration) electrolyzed at 5.0-5.3 v. and 49 amp. with the passage of 249 faradays (the initial concentration of starting material in mole-%, the potential applied in v., the average amp., and the total faradays of the various electrofluorination runs will be given throughout this abstract in parentheses in this order after the starting material) and the cell product fractionated gave 154 g. (CF₃)₂NCOF (II), b. 13-15°, 13% of the cell product consisted of a liquid, b. 38-41°, which was not identified, but yielded with MeOH a small yield of (CF₃)₂NCO₂Me (III).
 II treated with MeOH gave III, b. 76°, nD₂₅ 1.2997. A similar run with 2175 g. I (0.5, 5.0-5.3, 55, 452) gave 965 g. II. A run with 256 g. I in a 20-amp. cell yielded 174 g. II. Electrofluorination of 1139 g. HCONMe₂ (5.0, 5.2, 24.1, 198) gave 170 g. II, b. 15°, which treated with EtOH yielded (CF₃)₂NCO₂Et, b. 89°, nD₂₅ 1.3118. Et₂NCOCl (810 g.) (3.0, 5.2-5.4, 18.8, 100) gave similarly 730 g. crude product of which 33% boiled at 46-8° and 5% at 14-17°; the 46-8° fraction treated with 20% aqueous KOH or concentrated H₂SO₄ and refractionated yielded 273 g. CF₂O.CF₂.CF₂.NC₂F₅ (IV), b. 47.5°, nD₂₅ 1.2590, d₂₅ 1.685, MRD) 28.6. A similar run with 595 g. Et₂NCOCl (5.5, 4.6-4.8, 8, 125) yielded 40 g. II and 241 g. IV. Electrofluorination of 1176 g. Bu₂NCOCl (2.2, 5.2-5.4, 25.3, 184) gave 614 g. crude product of which 39% had b.p. 128-35°; the crude distillate treated with 25% aqueous base and fractionated yielded 211 g. CF₂O.CF(CF₃).CF₂.N-D₂₅ C₄F₉; b. 132.5°, nD₂₅ 1.2851, d₂₅ 1.809, MRD) 48.23; a possible impurity is (C₄F₉)₂NCF₃. Chloroformomorpholide (604 g.) (1.1, 4.8-5.0, 10, 170) gave similarly 750 g. crude product which was separated into 3 cuts: (1) overhead product, b. below 25°; (2) overhead product, b. above 25°; (3) cell drainings. Fraction 3 distilled gave no flats between 70 and 240°; distillation of fractions 1 and 2 yielded 34 g. II (converted with MeOH to III, b. 75-6°, nD₂₅ 1.3014), and 30 g. CF₂-CF₂O.CF₂.CF₂.NCOF, b. 45-8°. Electrofluorination of 569 g. CF₃CONMe₃ (-, 4.8-5.2, -, -) yielded 379 g. crude product which gave the following flats (b.p. and % of total given): (1) below -25°, 17; (2) 11-13.5°, 36; (3) 25-6°, 13. Fraction 1 gave 65 g. CF₃COF; fraction 2 yielded 137 g. II; fraction 3 refractionated gave 48 g. CF₃CON(CF₃)₂, b. 29.5-30°. A similar run with 196 g. (Me₂N)CCO (1.1, 4.6-4.9, 8, 56) gave 147 g. crude product which distilled yielded g. liquid, b. 15-20°, and 10 g. [(CF₃)₂N]CCO, b. 60-3°, nD₂₅ 1.2668; the low boiling cut gave 46 g. II. II passed at 575° over protruded Ni in a Ni tube and the system flushed with dry N for several hrs. gave 96% (89% conversion) CF₃N:CF₂, b. -33 to -31°, and 97% COF₂.
 ACCESSION NUMBER: 1957:12824 CAPLUS
 DOCUMENT NUMBER: 51:12824
 ORIGINAL REFERENCE NO.: 51:2737b-h
 TITLE: Fluorocarbon nitrogen compounds. I. Perfluorocarbamic acid derivatives, amides, and oxazolidines
 AUTHOR(S): Young, John A.; Simmons, Thomas C.; Hoffmann, Friedrich W.
 CORPORATE SOURCE: Univ. of Florida, Gainesville

L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
SOURCE: Journal of the American Chemical Society (1956), 78,
5637-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 51:12824

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	20.41	267.67
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.92	-2.92

FILE 'REGISTRY' ENTERED AT 15:57:00 ON 28 JAN 2005
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STRUCTURE FILE UPDATES: 27 JAN 2005 HIGHEST RN 821767-00-4
 DICTIONARY FILE UPDATES: 27 JAN 2005 HIGHEST RN 821767-00-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> s phosgene/cn
 L11 1 PHOSGENE/CN

=> d l11

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN

RN 75-44-5 REGISTRY

CN Carbonic dichloride (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Phosgene (8CI)

OTHER NAMES:

CN Carbon dichloride oxide

CN Carbon oxychloride

CN Carbonyl chloride

CN Carbonyl dichloride

CN CG

CN Chloroformyl chloride

CN Dichloroformaldehyde

CN Phosgen

FS 3D CONCORD

MF C C12 O

CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS,

BIOISIS,

BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,
CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHM, CSNB, DETHERM*, DIPPR*,
EMBASE, ENCOMPLIT, ENCOMPLITZ, ENCOMPAT, ENCOMPAT2, GMEIN*, HODOC*,
HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MCKK*, MSDS-OHS, NIOSHTIC,
PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT,
USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA Caplus document type: Book; Conference; Dissertation; Journal; Patent;

Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);

FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU

(Occurrence); PREP (Preparation); PROC (Process); PRP (Properties);

RACT

(Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological

study); PREP (Preparation); PROC (Process); PRP (Properties); RACT

(Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological

study); CMBI (Combinatorial study); FORM (Formation, nonpreparative);

MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC

(Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses);

NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical

study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP

(Preparation); PROC (Process); PRP (Properties); RACT (Reactant or

reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6883 REFERENCES IN FILE CA (1907 TO DATE)

267 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

6888 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN (Continued)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> s (oxalyl chloride)/cn
L12      1 (OXALYL CHLORIDE)/CN

=> d l12
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L12 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 79-37-8 REGISTRY
 CN Ethanedioyl dichloride (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Oxalyl chloride (6CI, 8CI)
 OTHER NAMES:
 CN Ethanedioyl chloride
 CN Oxalic acid chloride
 CN Oxalic acid dichloride
 CN Oxalic dichloride
 CN Oxaloyl chloride
 CN Oxaloyl dichloride
 CN Oxalyl dichloride
 FS 3D CONCORD
 MF C2 C12 O2
 CI COM
 LC STN Files: BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS,
 CASREACT,
 CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM*,
 EMBASE, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*,
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 USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
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 DT.CA Caplus document type: Conference; Dissertation; Journal; Patent;
 Report
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);
 MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP
 (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in
 record)
 RLD.P Roles for non-specific derivatives from patents: BIOL (Biological
 study); PREP (Preparation); PROC (Process); PRP (Properties); RACT
 (Reactant or reagent); USES (Uses)
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological
 study); CMBI (Combinatorial study); FORM (Formation, nonpreparative);
 OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP
 (Properties);
 RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
 RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical
 study); PREP (Preparation); PRP (Properties); RACT (Reactant or
 reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3148 REFERENCES IN FILE CA (1907 TO DATE)
 58 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 3156 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 49 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> fil casreact
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
13.74	281.41

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.92

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FILE CONTENT:1840 - 23 Jan 2005 VOL 142 ISS 4

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=>
Uploading C:\Program Files\Stnexp\Queries\10751824.str



chain nodes :
1 2 3 4 5 6 7 8
chain bonds :
1-2 2-3 4-5 4-6 5-7 5-8
exact/norm bonds :
1-2 2-3 4-5 5-7 5-8
exact bonds :
4-6

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS
fragments assigned product role:
containing 4
fragments assigned reactant/reagent role:

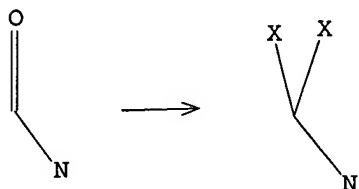
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L13 STRUCTURE UPLOADED

=> d query

L13

STR



Structure attributes must be viewed using STN Express query preparation.

=> s l13

SAMPLE SEARCH INITIATED 15:58:59 FILE 'CASREACT'

SCREENING COMPLETE - 26 REACTIONS TO VERIFY FROM 10 DOCUMENTS

100.0% DONE 26 VERIFIED 15 HIT RXNS 5 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 215 TO 825
PROJECTED ANSWERS: 5 TO 234

L14 5 SEA SSS SAM L13 (15 REACTIONS)

=> s l13 full

FULL SEARCH INITIATED 15:59:05 FILE 'CASREACT'

SCREENING COMPLETE - 564 REACTIONS TO VERIFY FROM 170 DOCUMENTS

100.0% DONE 564 VERIFIED 202 HIT RXNS 74 DOCS
SEARCH TIME: 00.00.01

L15 74 SEA SSS FUL L13 (202 REACTIONS)

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	106.96	388.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

FILE 'CAPLUS' ENTERED AT 15:59:12 ON 28 JAN 2005
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FILE COVERS 1907 - 28 Jan 2005 VOL 142 ISS 6
FILE LAST UPDATED: 27 Jan 2005 (20050127/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 115

L16 74 L15

=> s 75-44-5/rn

6885 75-44-5

267 75-44-5D

L17 6644 75-44-5/RN

(75-44-5 (NOTL) 75-44-5D)

=> s 116 and 117

L18 3 L16 AND L17

=> s 79-37-8/rn

3157 79-37-8

58 79-37-8D

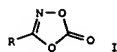
L19 3105 79-37-8/RN

(79-37-8 (NOTL) 79-37-8D)

=> s 116 and 119

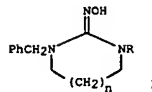
L20 0 L16 AND L19

=> d 118 1-3 abs ibib



AB 2-Perfluoroalkyl-1,3,4-dioxazol-2-ones (I, R = (CF₂)_nCF₃, n = 0, 2, 6) were prepared from RCONHOH and COCl₂. Pyrolysis of these dioxazolones gave good yields of RNCO, but the dioxazolones proved to be capriciously explosive.

ACCESSION NUMBER: 1983:558336 CAPLUS
DOCUMENT NUMBER: 99:158336
TITLE: 1,3,4-Dioxazol-2-ones: a potentially hazardous class of compounds
AUTHOR(S): Middleton, William J.
CORPORATE SOURCE: Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE, 19898, USA
SOURCE: Journal of Organic Chemistry (1983), 48(21), 3845-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:158336



AB Acyclic trisubstituted and previously unknown tetrasubstituted hydroxyguanidines RNMeC(:NOH)NR₁R₂ (R = Ph, PhCH₂; R₁ = Me, Et; R₂ = H, Me Et) were prepared from C-chloroformamidinium chlorides [RNMeCClNR₁R₂]⁺ (available from ureas or thioureas) via reaction with O-(tetrahydro-2-pyran-1-yl)hydroxylamine followed by acid hydrolysis of the protecting group.

Cyclic tri- and tetrasubstituted hydroxyguanidines I (R = Me, H; n = 0, 1) were prepared by the reaction of phosgene O-(tetrahydro-2-pyran-1-yl)oxime or phosgene O-(methylcarbamoyl)oxime with PhCH₂NH (C = H₂)nNHR, followed by acid or base hydrolysis of the protecting group.

ACCESSION NUMBER: 1976:542732 CAPLUS
DOCUMENT NUMBER: 85:142732
TITLE: Synthesis of cyclic and acyclic tri- and tetrasubstituted hydroxyguanidines
AUTHOR(S): Ziman, S. D.
CORPORATE SOURCE: Exp. Stn., E. I. du Pont de Nemours and Co., Wilmington, DE, USA
SOURCE: Journal of Organic Chemistry (1976), 41(20), 3253-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:142732

AB N-Monosubstituted formamides treated with COCl₂, yielded N,N'-disubstituted N-dichloromethylformamidinium chlorides, [Cl₂CHNRCH:NHR]Cl (I). The aliphatic I are relatively stable while the aromatic I are easily converted to the corresponding [RNH:CHNR]Cl (II). The reactions mechanisms are discussed. HCONHMe (147 g.) in 1000 cc. tetrahydrofuran treated at 30-5° within 2-3 hrs. with 255 g. COCl₂ in 300 cc. tetrahydrofuran (cooled to about -20°), heated 1 hr. at 35°, and cooled yielded 191 g. I (R = Me), m. 142-3° (decomposition). HCONHPr (17.4 g.) in 100 cc. tetrahydrofuran treated dropwise at 15° with 22.0 g. COCl₂ in 50 cc. tetrahydrofuran and cooled after 5 hrs. to -15° gave 16.2 g. I (R = Pr), m. 110-12° (decomposition). Iso-PrNHCHO (17.4 g.) in 60 cc. tetrahydrofuran treated at 5° with 20.0 g. COCl₂ in 40 cc. tetrahydrofuran and stirred 2 hrs. at 5-10° gave 16.5 g. I (R = iso-Pr) (III), m. 140-1° (decomposition). Iso-PrNHCHO (17.4 g.) in 30 cc. tetrahydrofuran added at -10° to 22.0 g. COCl₂ in 50 cc. tetrahydrofuran and stirred 1 hr. at 0° gave 17.0 g. III, m. 131-3°. Similarly were prepared the following I (R, % yield, and m.p. with decomposition given): iso-Bu, 87, 146-7° (a run with reversed addition of the reactants gave 55%, m. 148-9°); cyclohexyl, 86, 165-7°; cyclooctyl, 55, 156-7°; PhCH₂, 56, 116-18°; Ph (IV), 92, 112-14°; o-MeC₆H₄ (V), 64, 110-11°. IV recrystd. from Me₂CO-C₆H₆ gave II (R = Ph) (VI), m. 251-6° (decomposition). IV (20.0 g.) in 40 cc. Me₂CO and 60 cc. C₆H₆ heated gave 2.14 mole equivs. HCl and some CO. V recrystd. from Me₂CO-C₆H₆ yielded I (R = o-MeC₆H₄), m. 207-9° (decomposition). HCONHPh (72.6 g.) in 450 cc. tetrahydrofuran treated dropwise at 30-5° with 66.0 g. COCl₂ in 100 cc. cold tetrahydrofuran gave 48.0 g. VI, m. 250-2° (Me₂CO-C₆H₆). Similarly were prepared the following II (R, % yield, and m.p. given): m-MeC₆H₄, 55, 226-8° (Me₂CO); p-MeC₆H₄, 61, 246-8° (decomposition); p-MeOC₆H₄, 50, 253-5°; p-ETOC₆H₄, 68, 256-8°; m-ClC₆H₄, 55, 298-300°.

ACCESSION NUMBER: 1964:417916 CAPLUS
DOCUMENT NUMBER: 61:17916
ORIGINAL REFERENCE NO.: 61:2994a-e
TITLE: N-Monosubstituted formamide chlorides. I. Synthesis and properties of N,N'-disubstituted N-dichloromethylformamidinium chlorides
AUTHOR(S): Jentsch, Wolfgang
CORPORATE SOURCE: Badische Anilin- Soda-Fabrik A.-G., Ludwigshafen, Germany
SOURCE: Ber. (1964), 97(5), 1361-8
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:17916

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	ENTRY	SESSION
FULL ESTIMATED COST	17.76	406.13
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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FILE CONTENT:1840 - 23 Jan 2005 VOL 142 ISS 4

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L23      1 95:42254/AN
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=> d 123
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=> d 123 all

L23 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN
 AN 95:42254 CASREACT
 TI Preparation and study of difluoromethyl-substituted amines
 AU Allenstein, E.; Schrempf, G.
 CS Inst. Anorg. Chem., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
 SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1981), 474, 7-17
 CODEN: ZAACAB; ISSN: 0044-2313

DT Journal

LA German

CC 23-4 (Aliphatic Compounds)

Section cross-reference(s): 78

AB Fluorinating RN(CHCl₂)₂ (R = Me, Et) and N(CHCl₂)₃ with SbF₃ gave RN(CHF₂)₂ and N(CHF₂)₃, resp. Under certain conditions, MeN(CHO)₂ with COF₂ gave the known MeN(CHO)CHF₂. RN(CHF₂)₂ and N(CHF₂)₃ are mols. with covalent C-F bonds. Treating MeN(CHF₂)₂ with SbF₅ or BF₃ cleaved a F-

ion from a CHF₂ group to give [MeN(CHF₂):CHF]⁺ X⁻ (X = SbF₆ or BF₄).

ST fluorination chloromethyl amine; difluoromethylamine

IT Fluorination

(of bis(dichloromethyl)amines)

IT 7783-56-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorination by, of dichloromethyl amines)

IT 25891-29-6 66348-29-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorination of, with antimony trifluoride)

IT 815-55-4P 815-63-4P 73551-03-8P 78209-75-3P 78209-76-4P

78209-77-5P 78209-78-6P 78209-80-0P 78209-81-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 18197-25-6 66348-28-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with fluorinating agents)

IT 7789-23-3 14986-57-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with methylbis(dichloromethyl)amine)

IT 109-63-7 7783-70-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with methylbis(difluoromethyl)amine)

IT 353-50-4 7637-07-2, reactions 38078-09-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with methylidiforamide)

IT 7783-60-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with methylidiforamide or bis(dichloromethyl)amines)

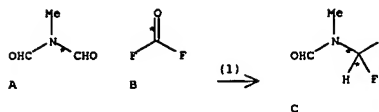
IT 71800-15-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sulfur tetrafluoride)

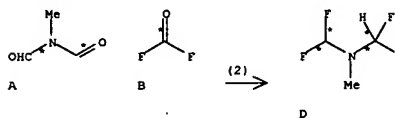
RX(1) OF 5 A + B ==> C

L23 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



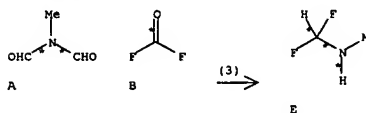
RX(1) RCT A 18197-25-6, B 353-50-4
 PRO C 78209-77-5

RX(2) OF 5 A + B ==> D



RX(2) RCT A 18197-25-6, B 353-50-4
 PRO D 78209-75-3

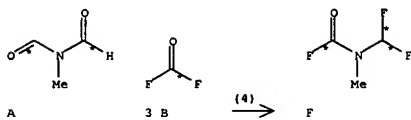
RX(3) OF 5 A + B ==> E



RX(3) RCT A 18197-25-6, B 353-50-4
 PRO E 78209-76-4

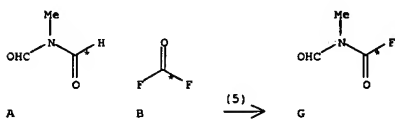
RX(4) OF 5 A + 3 B ==> F

L23 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



RX(4) RCT A 18197-25-6, B 353-50-4
 PRO F 815-63-4

RX(5) OF 5 A + B ==> G



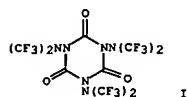
RX(5) RCT A 18197-25-6, B 353-50-4
 PRO G 815-55-4

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L25 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN
 AN 96:51430 CASREACT
 TI Reactions of bis(trifluoromethyl)carbamoyl fluoride with nucleophilic reagents
 AU Gontar, A. F.; Bykhovskaya, E. G.; Vinogradov, A. S.; Knunyants, I. L.
 CS Inst. Elementorg. Soedin. im. Nesmeyanova, Moscow, USSR
 SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1981), (11), 2632-5
 CODEN: IASKA6; ISSN: 0002-3353
 DT Journal
 LA Russian
 CC 21-2 (General Organic Chemistry)
 GI



AB (CF₃)₂NCOF (I) reacted with P(OR)₃ (R = Me, Et) to give F₂P(OR)₃ and CF₃N:CF₂ and further reactions of these species.
 ST carbamoyl fluoride trifluoromethyl reaction nucleophile; phosphite reaction trifluoromethylcarbamoyl fluoride; amine reaction trifluoromethylcarbamoyl fluoride; azide reaction trifluoromethylcarbamoyl fluoride; triazinetrione trifluoromethylamino; phosphorane trialkoxydifluoro

IT 371-71-1P
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in bis(trifluoromethyl)carbamoyl fluoride reactions with nucleophiles)

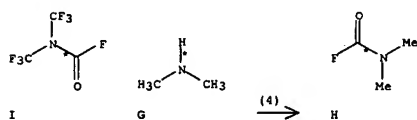
IT 358-74-7P 363-83-7P 431-14-1P 1813-18-9P 5954-50-7P 17167-31-6P
 17256-81-4P 17368-35-3P 55422-04-3P 66566-91-4P 66566-93-6P
 80567-54-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 109-89-7, reactions 121-45-9 122-52-1 124-40-3, reactions 26628-22-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with bis(trifluoromethyl)carbamoyl fluoride)
 IT 382-21-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with carbonyl fluoride)
 IT 353-50-4 432-00-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with nucleophiles)

RX(1) OF 34 ...A ==> B

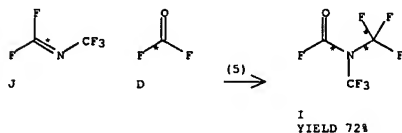
L25 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
 RX(3) RCT D 353-50-4, G 124-40-3
 PRO H 431-14-1

RX(4) OF 34 ...I + G ==> H



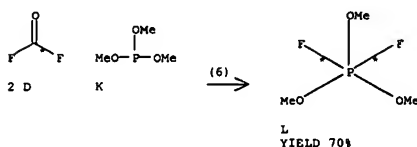
RX(4) RCT I 432-00-8, G 124-40-3
 PRO H 431-14-1

RX(5) OF 34 J + D ==> I...



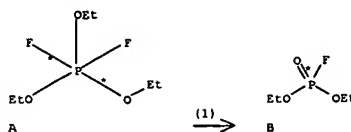
RX(5) RCT J 371-71-1, D 353-50-4
 RGT F 7789-23-3 KF
 PRO I 432-00-8

RX(6) OF 34 2 D + K ==> L...



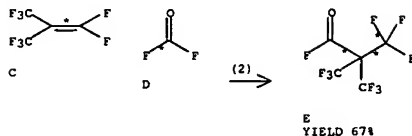
RX(6) RCT D 353-50-4, K 121-45-9
 PRO L 17167-31-6

L25 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



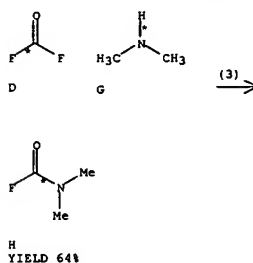
RX(1) RCT A 55422-04-3
 PRO B 358-74-7

RX(2) OF 34 C + D ==> E



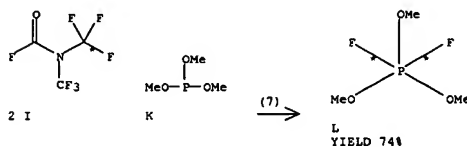
RX(2) RCT C 382-21-8, D 353-50-4
 RGT F 7789-23-3 KF
 PRO E 1813-18-9

RX(3) OF 34 D + G ==> H



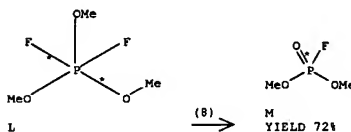
L25 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RX(7) OF 34 ...2 I + K ==> L...



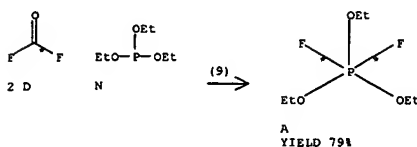
RX(7) RCT I 432-00-8, K 121-45-9
 PRO L 17167-31-6

RX(8) OF 34 ...L ==> M



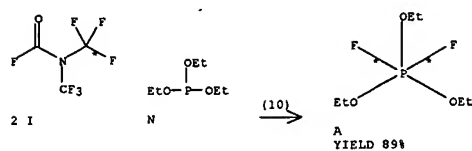
RX(8) RCT L 17167-31-6
 PRO M 5954-50-7

RX(9) OF 34 2 D + N ==> A...

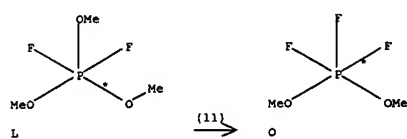


RX(9) RCT D 353-50-4, N 122-52-1
 PRO A 55422-04-3

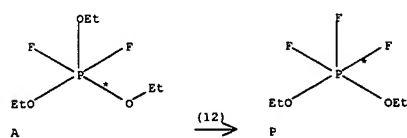
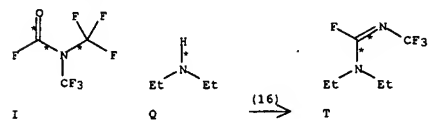
RX(10) OF 34 ...2 I + N ==> A...

RX(10) RCT I 432-00-8, N 122-52-1
PRO A 55422-04-3

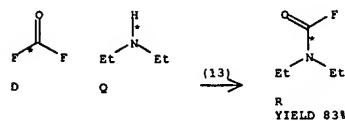
RX(11) OF 34 ...L ==> O

RX(11) RCT L 17167-31-6
PRO O 17368-35-3

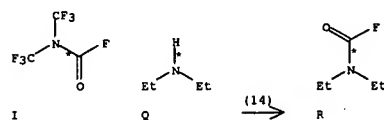
RX(12) OF 34 ...A ==> P

RX(12) RCT A 55422-04-3
PRO P 17256-81-4RX(16) RCT I 432-00-8, Q 109-89-7
PRO T 66566-93-6

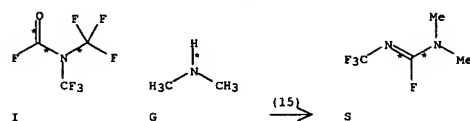
RX(13) OF 34 D + Q ==> R

RX(13) RCT D 353-50-4, Q 109-89-7
PRO R 363-83-7

RX(14) OF 34 ...I + Q ==> R

RX(14) RCT I 432-00-8, Q 109-89-7
PRO R 363-83-7

RX(15) OF 34 ...I + G ==> S

RX(15) RCT I 432-00-8, G 124-40-3
PRO S 66566-91-4

RX(16) OF 34 ...I + Q ==> T

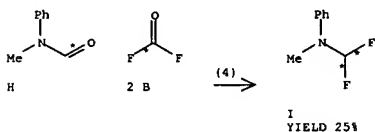
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L26 1 107:77261/AN
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L26 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS ON STN
 AN 107:77261 CASREACT
 TI Synthesis, vibrational spectra, and crystal structure analysis of di- and trifluoro-tetramethylammonium salts
 AU Brauer, D. J.; Buerger, H.; Grunwald, M.; Pawelke, G.; Wilke, J.
 CS Anorg. Chem., Univ. Gesamthochsch., Wuppertal, Fed. Rep. Ger.
 SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1986), 537, 63-78
 CODEN: ZAACAS; ISSN: 0044-2313
 DT Journal
 LA German
 CC 23-4 (Aliphatic Compounds)
 Section cross-reference(s): 75
 AB Tetramethylammonium salts, Me₃N+CH₂F (I), Me₃N+CHF₂ (II), and Me₃N+CF₃ (III), were prepared by quaternization of the corresponding fluoromethylamines. II was also generated from Me₃N and Zn-CF₂Br₂-KF in MeCN. I, II, and III were characterized by NMR and vibrational spectroscopy, a normal coordinate anal. being undertaken for III. The crystal structures of the iodides of II and III have been determined. In both cations the N-Me distances are on the average (II 1.508(2) Å; III 1.514(5) Å) longer than the N-CF valencies (II 1.497(4) Å; III 1.491(6) Å).
 ST fluoromethylamine prepn quaternization; formamide alkyl reaction carbonyl fluoride; fluoromethyltrimethylammonium prepn crystal structure; mol structure fluoromethyltriisopropylammonium; ammonium fluoromethyltrimethyl prepn crystal structure
 IT Quaternization (fluoromethylamines with Me iodide)
 IT Crystal structure Molecular structure (of fluoromethyltrimethylammonium iodides)
 IT Quaternary ammonium compounds, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, of fluoromethyltrimethylammonium iodides, crystal structure and)
 IT 25393-81-1P 109797-35-5P 109797-36-6P 109797-39-9P 109797-40-2P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and NMR of)
 IT 677-41-8P 25393-80-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and quaternization of)
 IT 109797-37-7P 109797-38-8P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, NMR, and crystal structure of)
 IT 683-81-8P 109797-33-3P 109797-34-4P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, NMR, and quaternization of, with Me iodide)
 IT 68-12-2P, Dimethylformamide, preparation 93-61-8P, Methylphenylformamide
 RL: PREP (Preparation) (reaction of, with carbonyl fluoride)
 IT 617-84-5, Diethylformamide 2700-30-3, Diisopropylformamide
 RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with carbonyl fluoride)
 IT 353-50-4, Carbonyl fluoride
 RL: RCT (Reactant); RACT (Reactant or reagent) (reactions of, with formamides)

L26 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS ON STN (Continued)

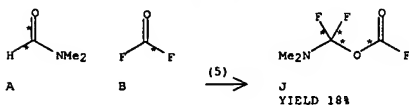
RX(3) RCT F 2700-30-3, B 353-50-4
 PRO G 109797-34-4

RX(4) OF 13 H + 2 B ==> I...



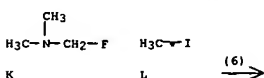
RX(4) RCT H 93-61-8, B 353-50-4
 PRO I 109797-35-5

RX(5) OF 13 A + B ==> J



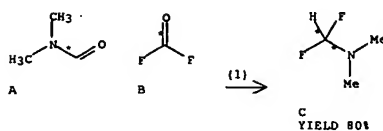
RX(5) RCT A 68-12-2, B 353-50-4
 PRO J 109797-36-6
 NTE excess COF₂

RX(6) OF 13 K + L ==> M



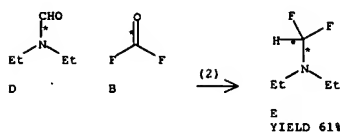
L26 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS ON STN (Continued)

RX(1) OF 13 A + B ==> C...



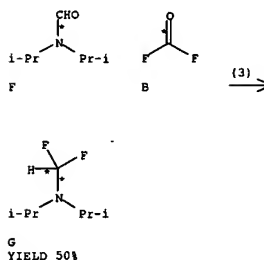
RX(1) RCT A 68-12-2, B 353-50-4
 PRO C 683-81-8

RX(2) OF 13 D + B ==> E...



RX(2) RCT D 617-84-5, B 353-50-4
 PRO E 109797-33-3

RX(3) OF 13 F + B ==> G



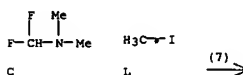
L26 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS ON STN (Continued)



• I⁻
 M
 YIELD 100%

RX(6) RCT K 25393-80-0, L 74-88-4
 PRO M 25393-81-1

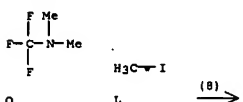
RX(7) OF 13 ...C + L ==> N



• I⁻
 N
 YIELD 100%

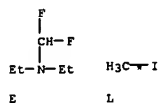
RX(7) RCT C 683-81-8, L 74-88-4
 PRO N 109797-37-7

RX(8) OF 13 O + L ==> P



● I⁻P
YIELD 100%RX(8) RCT O 677-41-8, L 74-88-4
PRO P 109797-38-8

RX(9) OF 13 ...E + L ==> Q



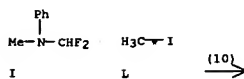
E

L

(9) →

● I⁻Q
YIELD 100%RX(9) RCT E 109797-33-3, L 74-88-4
PRO Q 109797-39-9

RX(10) OF 13 ...I + L ==> R



I

H3C-I
L

(10) →

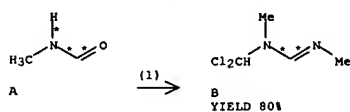
● I⁻R
YIELD 100%RX(10) RCT I 109797-35-5, L 74-88-4
PRO R 109797-40-2

=> s 61:17916/an
L27 1 61:17916/AN
=> d l27 all

L27 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN
 AN 61:17916 CASREACT
 TI N-Monosubstituted formamide chlorides. I. Synthesis and properties of
 N,N'-disubstituted N-dichloromethylformamidinium chlorides
 AU Jentsch, Wolfgang
 CS Badische Anilin- Soda-Fabrik A.-G., Ludwigshafen, Germany
 SO Ber. (1964), 97(5), 1361-8
 DT Journal
 LA Unavailable
 CC 35 (Noncondensed Aromatic Compounds)
 AB N-Monosubstituted formamides treated with COCl₂, yielded
 N,N'-disubstituted N-dichloromethylformamidinium chlorides,
 [Cl₂CHN(R)CH:NHR]Cl (I). The aliphatic I are relatively stable while the
 aromatic I are easily converted to the corresponding [R₂N:CHNHR]Cl (II).
 The reactions mechanisms are discussed. HCONHMe (147 g.) in 1000 cc.
 tetrahydrofuran treated at 30-5° within 2-3 hrs. with 255 g. COCl₂
 in 300 cc. tetrahydrofuran (cooled to about -20°), heated 1 hr. at
 35°, and cooled yielded 191 g. I (R = Me), m. 142-3°
 (decomposition). HCONHPr (17.4 g.) in 100 cc. tetrahydrofuran treated
 dropwise
 at 15° with 22.0 g. COCl₂ in 50 cc. tetrahydrofuran and cooled
 after 5 hrs. to -15° gave 16.2 g. I (R = Pr), m. 110-12°
 (decomposition). Iso-PrNHCHO (17.4 g.) in 60 cc. tetrahydrofuran
 treated at
 5° with 20.0 g. COCl₂ in 40 cc. tetrahydrofuran and stirred 2 hrs.
 at 5-10° gave 16.5 g. I (R = iso-Pr) (III), m. 140-1°
 (decomposition). Iso-PrNHCHO (17.4 g.) in 30 cc. tetrahydrofuran added
 at
 -10° to 22.0 g. COCl₂ in 50 cc. tetrahydrofuran and stirred 1 hr.
 at 0° gave 17.0 g. III, m. 131-3°. Similarly were prepared
 the following I (R, % yield, and m.p. with decomposition given): iso-Bu,
 87, 146-7° (a run with reversed addition of the reactants gave 55%, m.
 148-9°); cyclohexyl, 86, 165-7°; cyclooctyl, 55,
 156-7°; PhCH₂, 56, 116-18°; Ph (IV), 92, 112-14°; o-MeC₆H₄
 (V), 64, 110-11°. IV recrystd. from Me₂CO·C₆H₆ gave II (R = Ph)
 (VI), m. 251-6° (decomposition). IV (20.0 g.) in 40 cc. Me₂CO and 60
 cc. C₆H₆ heated gave 2.14 mole equivs. HCl and some CO. V recrystd. from
 Me₂CO·C₆H₆ yielded I (R = o-MeC₆H₄), m. 207-9° (decomposition). HCONHPh
 (72.6 g.) in 450 cc. tetrahydrofuran treated dropwise at 30-5° with
 66.0 g. COCl₂ in 100 cc. cold tetrahydrofuran gave 48.0 g. VI, m.
 250-2° (Me₂CO·C₆H₆). Similarly were prepared the following II (R, %
 yield, and m.p. given): m-MeC₆H₄, 55, 226-8° (Me₂CO); p-MeC₆H₄, 61,
 246-8° (decomposition); p-MeOC₆H₄, 50, 253-5°; p-EOC₆H₄, 68,
 256-8°; m-ClC₆H₄, 55, 298-300°.
 IT 463-72-9, Carbamoyl chloride
 (derivs., hydrochlorides)
 IT 57-13-6, Urea
 (derivs., reaction with COCl₂, mechanism of)
 IT 3892-95-3, Carbanilide, N,N'-dichloro-2,2'-dimethyl-4,4'-dinitro-
 3892-96-4, Carbanilide, N,N'-dichloro-4,4'-dinitro- 20868-98-8,
 Formamidine, N,N'-diphenyl-, hydrochloride 55002-70-5, Formamidine,
 N,N'-di-p-tolyl-, hydrochloride 66348-31-0, Formamidine,
 N-(dichloromethyl)-N,N'-dimethyl-, hydrochloride 91692-96-5,
 Carbanilide, 4,4'-dibromo-N,N',2,2',6,6'-hexachloro- 91692-97-6,
 Carbanilide, 2,2',4,4',6,6'-hexabromo-N,N'-dichloro- 91693-01-5,
 Carbanilide, N,N',2,2',6,6'-hexachloro-4,4'-dinitro- 91693-24-2,
 Carbanilide, 2,2',6,6'-tetrabromo-N,N'-dichloro- 93335-19-4,
 Formamidine, N-(dichloromethyl)-N,N'-dipropyl-, hydrochloride
 93335-20-7, Formamidine, N-(dichloromethyl)-N,N'-diisopropyl-,

L27 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
 hydrochloride 96634-98-9, Formamidine, N-(dichloromethyl)-N,N'-
 diisobutyl-, hydrochloride 96985-07-8, Formamidine, N-(dichloromethyl)-
 N,N'-diphenyl-, hydrochloride 97216-23-4, Formamidine,
 N,N'-di-o-tolyl-,
 hydrochloride 97282-74-1, Formamidine, N,N'-dicyclohexyl-N-
 (dichloromethyl)-, hydrochloride 97377-89-4, Formamidine,
 NN'-di-m-tolyl-, hydrochloride 97377-97-4, Formamidine,
 N,N-bis(p-methoxyphenyl)-, hydrochloride 97754-65-9, Formamidine,
 N-(dichloromethyl)-N,N'-di-o-tolyl-, hydrochloride 97769-04-5,
 Formamidine, N,N'-dibenzyl-N-(dichloromethyl)-, hydrochloride
 100456-87-9, Formamidine, N,N'-dicyclooctyl-N-(dichloromethyl)-,
 hydrochloride
 (prepn. of)
 IT 75-44-5, Phosgene
 (reactions of, with ureas)
 IT 75-44-5, Phosgene
 (reactions of, with N-substituted formamides)
 IT 75-12-7, Formamide
 (N-derivs., reaction with COCl₂)

RX(1) OF 1 A ==> B



RX(1) RCT A 123-39-7
 RGT C 7646-79-9 CoCl₂
 PRO B 66329-88-2
 SOL 109-99-9 THF
 NTE Classification: Isomerisation; Chlorination; Condensation; #
 Conditions: COCl₂; THF; -30 deg 2-3h

```
=> fil casreacat
'CASREACAT' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'CASREACT'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available. If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.
```

```
=> fil casreat
'CASREAT' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'CASREACT'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available. If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.
```

```
=> fil casreact
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                               ENTRY      SESSION
FULL ESTIMATED COST          39.27      445.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                               ENTRY      SESSION
CA SUBSCRIBER PRICE          -2.72      -7.83
```

FILE 'CASREACT' ENTERED AT 16:10:07 ON 28 JAN 2005
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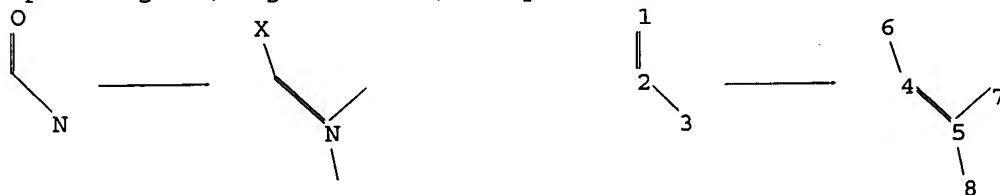
FILE CONTENT:1840 - 23 Jan 2005 VOL 142 ISS 4

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*****
*                                     *
*   CASREACT now has more than 8 million reactions   *
*                                     *
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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Uploading C:\Program Files\Stnexp\Queries\10751824.str
```



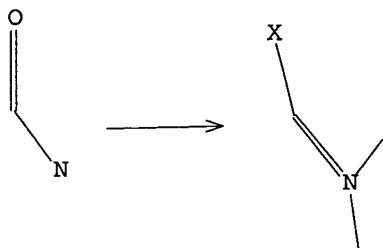
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1 2 3 4 5 6 7 8
chain bonds :
1-2 2-3 4-5 4-6 5-7 5-8
exact/norm bonds :
1-2 2-3 4-5 5-7 5-8
exact bonds :
4-6

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS
fragments assigned product role:
containing 4
fragments assigned reactant/reagent role:
containing 1

L28 STRUCTURE UPLOADED

=> d query

L28 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l28

SAMPLE SEARCH INITIATED 16:11:32 FILE 'CASREACT'

SCREENING COMPLETE - 124 REACTIONS TO VERIFY FROM 35 DOCUMENTS

100.0% DONE 124 VERIFIED 8 HIT RXNS 5 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 1812 TO 3148

PROJECTED ANSWERS: 5 TO 234

L29 5 SEA SSS SAM L28 (8 REACTIONS)

=> s l28 full

FULL SEARCH INITIATED 16:11:37 FILE 'CASREACT'

SCREENING COMPLETE - 2793 REACTIONS TO VERIFY FROM 570 DOCUMENTS

100.0% DONE 2793 VERIFIED 80 HIT RXNS 47 DOCS
SEARCH TIME: 00.00.01

L30 47 SEA SSS FUL L28 (80 REACTIONS)

=> d his

(FILE 'HOME' ENTERED AT 15:50:09 ON 28 JAN 2005)

FILE 'CASREACT' ENTERED AT 15:50:21 ON 28 JAN 2005

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 47 S L1 FULL

FILE 'REGISTRY' ENTERED AT 15:51:29 ON 28 JAN 2005

L4 1 S (OXALYL FLUORIDE)/CN

L5 1 S DIFLUOROPHOSGENE/CN

FILE 'CAPLUS' ENTERED AT 15:53:45 ON 28 JAN 2005

L6 47 S L3

L7 1252 S 353-50-4/RN

L8 4 S L6 AND L7

L9 154 S 359-40-0/RN

L10 0 S L6 AND L9

FILE 'REGISTRY' ENTERED AT 15:57:00 ON 28 JAN 2005

L11 1 S PHOSGENE/CN

L12 1 S (OXALYL CHLORIDE)/CN

FILE 'CASREACT' ENTERED AT 15:58:04 ON 28 JAN 2005

L13 STRUCTURE UPLOADED

L14 5 S L13

L15 74 S L13 FULL

FILE 'CAPLUS' ENTERED AT 15:59:12 ON 28 JAN 2005

L16 74 S L15

L17 6644 S 75-44-5/RN

L18 3 S L16 AND L17

L19 3105 S 79-37-8/RN

L20 0 S L16 AND L19

FILE 'CASREACT' ENTERED AT 16:02:29 ON 28 JAN 2005

L21 0 S 95:42254/DN

L22 0 S 95:42254

L23 1 S 95:42254/AN

L24 0 S 96:51430

L25 1 S 96:51430/AN

L26 1 S 107:77261/AN

L27 1 S 61:17916/AN

FILE 'CASREACT' ENTERED AT 16:10:07 ON 28 JAN 2005

L28 STRUCTURE UPLOADED

L29 5 S L28

L30 47 S L28 FULL

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

107.39

552.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.83

FILE 'CAPLUS' ENTERED AT 16:11:51 ON 28 JAN 2005
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FILE COVERS 1907 - 28 Jan 2005 VOL 142 ISS 6
 FILE LAST UPDATED: 27 Jan 2005 (20050127/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l30
L31      47 L30

=> s l31 and l7
L32      0 L31 AND L7

=> s l31 and l9
L33      0 L31 AND L9

=> s l31 and l17
L34      3 L31 AND L17

=> s l31 and l19
L35      6 L31 AND L19

=> s l34 or l35
L36      9 L34 OR L35

=> d l36 1-9 abs ibib
```

L36 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 AB 1,8-Bis(tetramethylguanidino)naphthalene (TMGN) is a new, readily accessible, and stable "proton sponge" with an exptl. pK_{BH}⁺ value of 25.1 in MeCN, which is nearly seven orders of magnitude higher in basicity than the classical proton sponge 1,8-bis(dimethylamino)naphthalene (DMAN). Because of the sterically less crowded character of the proton-accepting sp²-nitrogen atoms, TMGN also has a higher kinetic basicity than DMAN, which is shown by time-resolved proton self-exchange reactions. TMGN is more resistant to hydrolysis and is a weaker nucleophile towards the alkylating agent EtI in comparison to the com. available guanidine 7-methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (MTBD). Crystal structures of the free base, of the mono- and bis-protonated base were determined.

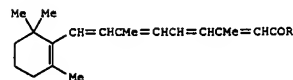
The dynamic behavior of all three species in solution was investigated by variable-temperature 1H NMR expts. ΔG_{thermod.} values obtained by spectra simulation reveal a concerted mechanism of rotation about the C-N bonds of the protonated forms of TMGN.

ACCESSION NUMBER: 2002:290351 CAPLUS
 DOCUMENT NUMBER: 137:109017
 TITLE: 1,8-bis(tetramethylguanidino)naphthalene (TMGN): a new, superbasic and kinetically active "proton sponge"
 AUTHOR(S): Raab, Volker; Kipke, Jennifer; Gschwind, Ruth M.; Sundermeyer, Jorg
 CORPORATE SOURCE: Fachbereich Chemie, Philipps-Universitat Marburg, Marburg, 35032, Germany
 SOURCE: Chemistry--A European Journal (2002), 8(7), 1682-1693
 CODEN: CEUJED; ISSN: 0947-6539
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:109017
 REFERENCE COUNT: 126 THERE ARE 126 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L36 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Single diastereomers of tris(α-methylbenzyl)amine were efficiently synthesized in either racemic [(2)-1] or optically pure (1) form starting from α-methylbenzylamine. The X-ray crystal structures reveal virtually flat nitrogen centers.

ACCESSION NUMBER: 2000:887383 CAPLUS
 DOCUMENT NUMBER: 134:237243
 TITLE: Synthesis of the novel amine (R^{*},R^{*},R^{*})-tris(α-methylbenzyl)amine. X-Ray crystal structures of racemic and enantiomerically pure forms
 AUTHOR(S): Wyatt, Paul; Butts, Craig P.; Patel, Vipulkumar; Voysey, Ben
 CORPORATE SOURCE: School of Chemistry, Cantock's Close, Bristol, BS8 1TS, UK
 SOURCE: Perkin 1 (2000), (24), 4222-4223
 CODEN: PERKF9; ISSN: 1470-4358
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:237243
 REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L36 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 GI



AB (all-trans)-Retinoyl chloride (I; R = Cl) (II) is prepared by chlorination of (all-trans)-retinoic acid (II; R = OH) (III) with Me₂N+CHCl₂ (IV) under mild conditions. Degassed dry DMF was treated with oxalyl chloride in Et₂O to give a white precipitate IV, which was stirred with a slurry of acid III in DMF at room temperature to give II, which was treated with aniline derivs. to give the corresponding retinamides.

ACCESSION NUMBER: 1989:135536 CAPLUS
 DOCUMENT NUMBER: 110:135536
 TITLE: Process for preparing retinoyl chlorides
 INVENTOR(S): Maryanoff, Cynthia Anne
 PATENT ASSIGNEE(S): McNeilab, Inc., USA
 SOURCE: Eur. Pat. Appl., 7 pp.
 CODEN: EPXKDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 261911	A2	19880330	EP 1987-308333	19870921
EP 261911	A3	19880601		
EP 261911	B1	19910821		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4743400	A	19880510	US 1986-909794	19860922
JP 63119456	A2	19880524	JP 1987-235043	19870921
JP 07107044	B4	19951115		
HU 45009	A2	19880530	HU 1987-4254	19870921
HU 201523	B	19901128		
CA 1278310	A1	19901227	CA 1987-547388	19870921
AT 66471	E	19910915	AT 1987-308333	19870921
PRIORITY APPLN. INFO.:			US 1986-909794	A 19860922
			EP 1987-308333	A 19870921

OTHER SOURCE(S): CASREACT 110:135536

L36 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The title chlorocarbenium ions RR1C+Cl SbCl6⁻ (I; R = Me₂N, R₁ = H, Me₂N, Ph, 4-MeC₆H₄) were treated with NH₄SCN in liquid SO₂ to give 51-97% azabutatrienium salts RR1C=N⁺:C:S SbCl6⁻. Reaction of I (R = Me₂N, R₁ = H; R = R₁ = Ph, 4-MeOC₆H₄, etc.) with KOCCN in the presence of ketones R₂R₃CO (R₂ = Ph, R₃ = Ph, 4-MeOC₆H₄; R₂ = R₃ = 4-ClC₆H₄, 4-MeOC₆H₄, etc.) gave 61-81% azallenium salts RR1C=N⁺:C:R₂R₃ SbCl6⁻. Treatment of (4-ClC₆H₄)₂CCl₂ with 2 equiv of NH₄SCN gave 97% (4-ClC₆H₄)₂C(SCN)₂ which rearranged in refluxing CH₂Cl₂ to give 98% (4-ClC₆H₄)₂C(NCS)₂.

ACCESSION NUMBER: 1988:167083 CAPLUS
 DOCUMENT NUMBER: 108:167083
 TITLE: On the reactions of α-chlorocarbenium ions with ammonium thiocyanate and potassium cyanate
 AUTHOR(S): Hamed, Atef; Mueller, Edgar; Al-Talib, Mahmoud; Jochims, Johannes C.
 CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
 SOURCE: Synthesis (1987), (8), 745-8
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:167083

L36 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 AB (E)-3,5,4-RR1(HO)C6H2CH:CHCO2H (I; R = H, R1 = H, MeO, HO; R = R1 = MeO) are esterified in 40-80% yield with PhSK or PhSH after activation by Me2N+:CHCl Cl- or 2-fluoro-N-methylpyridinium p-tosylate resp. Prior protection of the aromatic OH is unnecessary; competitive Michael addition does not occur. Transesterification with CoA gives 30-50% thiocinnamates of biol. interest.
 ACCESSION NUMBER: 1988:21429 CAPLUS
 DOCUMENT NUMBER: 108:21429
 TITLE: Synthesis of S-phenyl p-hydroxythiocinnamates as precursors of S-CoA esters
 AUTHOR(S): Duran, Elisabeth; Duran, Hubert; Cezaux, Louis; Gorrichon, Lilliane; Tisnes, Pierre; Sarni, Farid
 CORPORATE SOURCE: Cent. Physiol. Veg., Univ. Paul Sabatier, Toulouse, 31062, Fr.
 SOURCE: Bulletin de la Societe Chimique de France (1987), (1), 143-8
 CODEN: BSCFAS; ISSN: 0037-8968
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 OTHER SOURCE(S): CASREACT 108:21429

L36 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Sterically-hindered tertiary amines R21CHNR2 (R = Me2CH or cyclohexyl, R1 = alkyl, Ph), R3CH2CHR2CH2N(CHMe2)2 (R2 = Me, R3 = H; R2R3 = (CH2)4) and CH3CH2CH(CMe3)N(CHMe2)2 were prepared by reaction of iminium salts (e.g., ClCH = N+R2Cl-) with Grignard or alkyllithium compds. hindered guanidines [(Me2CH)2N]2C:NCHNR4R5 (R4, R5 = Me, Et) were also prepared The pKa values of the amines and guanidines were determined and their alkylation with FSO3Me was studied.
 ACCESSION NUMBER: 1986:33742 CAPLUS
 DOCUMENT NUMBER: 104:33742
 TITLE: Synthesis and properties of sterically hindered tertiary amines and guanidines
 AUTHOR(S): Wisland, Gerhard; Simchen, Gerhard
 CORPORATE SOURCE: Inst. Org. Chem. Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
 SOURCE: Liebigs Annalen der Chemie (1985), (11), 2178-93
 CODEN: LACHDL; ISSN: 0170-2041
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 104:33742

L36 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Acetic acids RCH2CO2H (R = Me, PhCH2, Me2CH, cyclobutyl) treated with (Me2CH)2NHLi and then Me2N+:CHOMe MeSO4- underwent decarboxylative double formylation at or below 50-60° to yield malonaldehydes RCH(CHO)2 (I). Other I (R = mesityl, Ph, 2-thienyl, Me3C, 1-adamantyl) were obtained by treating enamines RCH:CHNR12 (R12N = Me2N, morpholino) (prepared from RCH2CO2H) with Vilsmeier reagents R12N+:CHCl Cl-.
 ACCESSION NUMBER: 1984:138209 CAPLUS
 DOCUMENT NUMBER: 100:138209
 TITLE: Malonaldehyde derivatives: a general one- or two-step synthesis from substituted acetic acids
 AUTHOR(S): Knorr, Rudolf; Loew, Peter; Hassel, Petra; Bronberger, Hildegard
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Munich, Munich, D-8000/2, Fed. Rep. Ger.
 SOURCE: Journal of Organic Chemistry (1984), 49(7), 1288-90
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 100:138209

L36 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Me2NCHCl:N+Me2 Cl- reacted smoothly with a variety of carboxylic and phosphoric acids in the presence of a tertiary amine to give the corresponding acid anhydrides in high yields. The reactions were generally carried out in CH2Cl2 at -30° with warming to 0° or room temperature
 ACCESSION NUMBER: 1984:102367 CAPLUS
 DOCUMENT NUMBER: 100:102367
 TITLE: One-pot synthesis of acid anhydrides from acids using N,N,N',N'-tetramethylchloroformamidinium chloride under mild conditions
 AUTHOR(S): Fujisawa, Tamotsu; Tajima, Kazuhisa; Sato, Toshio
 CORPORATE SOURCE: Chem. Dep. Resour., Mie Univ., Tsu, 514, Japan
 SOURCE: Bulletin of the Chemical Society of Japan (1983), 56(11), 3529-30
 CODEN: BCSJAB; ISSN: 0009-2673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 100:102367

L36 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
AB The carboxyl group was selectively reduced to the hydroxymethyl group by
Me₂N⁺:CHCl⁻ and NaBH₄, even in the presence of halide, ester, nitrile,
and olefin moieties.
ACCESSION NUMBER: 1983:504431 CAPLUS
DOCUMENT NUMBER: 99:104431
TITLE: Chemoselective reduction of carboxylic acids into
alcohols using N,N-dimethylchloromethyleniminium
chloride and sodium borohydride
AUTHOR(S): Fujisawa, Tamotsu; Mori, Toshiki; Sato, Toshio
CORPORATE SOURCE: Chem. Dep. Resour., Mie Univ., Tsu, 514, Japan
SOURCE: Chemistry Letters (1983), (6), 835-8
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:104431

=> d his

(FILE 'HOME' ENTERED AT 15:50:09 ON 28 JAN 2005)

FILE 'CASREACT' ENTERED AT 15:50:21 ON 28 JAN 2005

L1 STRUCTURE UPLOADED
L2 1 S L1
L3 47 S L1 FULL

FILE 'REGISTRY' ENTERED AT 15:51:29 ON 28 JAN 2005

L4 1 S (OXALYL FLUORIDE)/CN
L5 1 S DIFLUOROPHOSGENE/CN

FILE 'CAPLUS' ENTERED AT 15:53:45 ON 28 JAN 2005

L6 47 S L3
L7 1252 S 353-50-4/RN
L8 4 S L6 AND L7
L9 154 S 359-40-0/RN
L10 0 S L6 AND L9

FILE 'REGISTRY' ENTERED AT 15:57:00 ON 28 JAN 2005

L11 1 S PHOSGENE/CN
L12 1 S (OXALYL CHLORIDE)/CN

FILE 'CASREACT' ENTERED AT 15:58:04 ON 28 JAN 2005

L13 STRUCTURE UPLOADED
L14 5 S L13
L15 74 S L13 FULL

FILE 'CAPLUS' ENTERED AT 15:59:12 ON 28 JAN 2005

L16 74 S L15
L17 6644 S 75-44-5/RN
L18 3 S L16 AND L17
L19 3105 S 79-37-8/RN
L20 0 S L16 AND L19

FILE 'CASREACT' ENTERED AT 16:02:29 ON 28 JAN 2005

L21 0 S 95:42254/DN
L22 0 S 95:42254
L23 1 S 95:42254/AN
L24 0 S 96:51430
L25 1 S 96:51430/AN
L26 1 S 107:77261/AN
L27 1 S 61:17916/AN

FILE 'CASREACT' ENTERED AT 16:10:07 ON 28 JAN 2005

L28 STRUCTURE UPLOADED
L29 5 S L28
L30 47 S L28 FULL

FILE 'CAPLUS' ENTERED AT 16:11:51 ON 28 JAN 2005

L31 47 S L30
L32 0 S L31 AND L7
L33 0 S L31 AND L9
L34 3 S L31 AND L17
L35 6 S L31 AND L19
L36 9 S L34 OR L35

=> s 17 and 19

L37 35 L7 AND L9

=> d l37 1-35 abs ibib

L37 ANSWER 1 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB This invention describes a method for processing an article with a dense processing fluid in a processing chamber while applying ultrasonic energy during processing. The dense fluid may be generated in a sep. pressurization vessel and transferred to the processing chamber, or alternatively may be generated directly in the processing chamber. A processing agent may be added to the pressurization vessel, to the processing chamber, or to the dense fluid during transfer from the pressurization vessel to the processing chamber. The ultrasonic energy may be generated continuously at a constant frequency or at variable frequencies. Alternatively, the ultrasonic energy may be generated intermittently.

ACCESSION NUMBER: 2004:609574 CAPLUS
 DOCUMENT NUMBER: 141:149433
 TITLE: Processing of semiconductor components with dense processing fluids and ultrasonic energy
 INVENTOR(S): McDermott, Wayne Thomas; Subawalla, Hoshang; Johnson, Andrew David; Schwarz, Alexander
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 25 pp., Cont.-in-part of U.S. Ser. No. 253,054.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004144399	A1	20040729	US 2003-737458	20031216
US 2004055621	A1	20040325	US 2002-253054	20020924
PRIORITY APPLN. INFO.:			US 2002-253054	A2 20020924

L37 ANSWER 3 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Two-, three-, and four-bond 19F-19F spin-spin coupling consts. (nJFF) for a set of small fluoro-substituted organic mols. have been computed using
 ab initio equation-of-motion coupled cluster singles and doubles (EOM-CCSD) theory. The computed values reproduce the exptl. signs and magnitudes of nJFF. The straight line that relates the exptl. and computed coupling consts. has a slope of approx. 1 and passes through the point (0, 0 Hz) within the uncertainties of the fit. Hence, EOM-CCSD values of nJFF should be excellent predictors of exptl. values when these are not available. All of the components of nJFF except for the diamagnetic spin-orbit term may be large and must be evaluated if agreement between theory and experiment is to be obtained.

ACCESSION NUMBER: 2004:55315 CAPLUS
 DOCUMENT NUMBER: 140:320957
 TITLE: Computed EOM-CCSD 19F-19F spin-spin coupling constants
 AUTHOR(S): in small organic molecules
 CORPORATE SOURCE: Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose
 SOURCE: Department of Chemistry, Youngstown State University, Youngstown, OH, 44555, USA
 CODEN: ZPCFAX; ISSN: 0942-9352
 PUBLISHER: Oldenbourg Wissenschaftsverlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L37 ANSWER 2 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB R1CF2NR2R3 (R1 = H, C1-12 alkyl, C3-14 aryl, etc.; R2, R3 = C1-12 alkyl, C3-14 aryl, C4-15 aralkyl; R1R2 or R1R3 can form C3-16 carbocyclic ring), agents for fluorination of alcs. and carbonyl compds., especially ketones, carboxylic acids and aldehydes, were prepared with improved yields and without taking special precautionary measures by reacting carbonyl compds. R1CONR2R3 (R1-R2 as above) with (COF)2 or COF2 in a solvent. For example, adding cooled (COF)2 to CH2Cl2 solution of Me3CCONMe2 at -10° in a closed steel reactor and stirring the mixture at room temperature and for 16 h at 40° gave 93% Me3CCF2NMe2 as light yellow liquid

ACCESSION NUMBER: 2004:564132 CAPLUS
 DOCUMENT NUMBER: 141:125376
 TITLE: Manufacture of α,α -difluoramines and difluoromethylene- α,α -diazo compounds as fluorination agents
 INVENTOR(S): Ebenbeck, Wolfgang; Marhold, Albrecht; Kolomeitsev, Alexander; Roeschenthaler, Gerd-Volker
 PATENT ASSIGNEE(S): Bayer A.-G., Germany
 SOURCE: Ger. Offen., 6 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10300113	A1	20040715	DE 2003-10300113	20030107
EP 1439170	A1	20040721	EP 2003-29973	20031230
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004198975	A1	20041007	US 2004-751824	20040105
JP 2004210792	A2	20040729	JP 2004-1699	20040107
PRIORITY APPLN. INFO.:			DE 2003-10300113	A 20030107

OTHER SOURCE(S): MARPAT 141:125376

L37 ANSWER 4 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The invention relates to a method and apparatus for atomic layer deposition with reactive gas species generated at the point of use, which permits the cycling of the system through a number of on/off states at a fast rate for higher processing throughput. The apparatus has a dispenser unit used to prevent mixing of a precursor gas and an input gas. From the dispenser unit, a flow of the input gas is provided over a surface of the workpiece where a beam of the electromagnetic radiation is directed into the input gas in close proximity to the surface of the workpiece, but spaced a finite distance from the surface. The input gas is dissociated by the beam producing a high flux point of use generated reactive gas species that reacts with a surface reactant formed on the surface of the workpiece by a direct flow of the precursor gas flown from the dispensing unit. The surface reactant and reactive gas species react to form a desired monolayer of a material on the surface of the workpiece.

ACCESSION NUMBER: 2003:717539 CAPLUS
 DOCUMENT NUMBER: 139:238716
 TITLE: Method and apparatus for atomic layer deposition with reactive gas species generated at the point of use
 INVENTOR(S): Sandhu, Gurtej S.
 PATENT ASSIGNEE(S): Micron Technology, Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 13 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003170389	A1	20030911	US 2002-91938	20020305
US 6730367	B2	20040504		
US 2004083951	A1	20040506	US 2003-697511	20031030
US 2004185184	A1	20040923	US 2004-765314	20040127
PRIORITY APPLN. INFO.:			US 2002-91938	A3 20020305

L37 ANSWER 5 OF 35 CAPLUS COPYRIGHT 2005 ACS ON STN
 AB The invention relates to a method and system for providing high flux of point of use activated reactive species for semiconductor processing. A workpiece is exposed to a gaseous atmosphere containing a transmission gas that is nonattenuating to preselected wavelengths of electromagnetic radiation.
 A laminar flow of a gaseous constituent is also provided over a planar surface of the workpiece, where a beam of the electromagnetic radiation is directed into the gaseous atmosphere such that it converges in the laminar flow to provide maximum beam energy in close proximity to the surface of the workpiece, but spaced a finite distance from the workpiece. The gaseous constituent is dissociated by the beam producing an activated reactive species that reacts with the surface of the workpiece.
 ACCESSION NUMBER: 2003:434954 CAPLUS
 DOCUMENT NUMBER: 138:394347
 TITLE: Method and system for providing high flux of point of use activated reactive species for semiconductor processing
 INVENTOR(S): Sandhu, Gurtej S.; Doan, Trung T.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 11 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003102008	A1	20030605	US 2001-998073	20011130
US 2004020511	A1	20040205	US 2003-392940	20030320
US 6793736	B2	20040921		

 PRIORITY APPLN. INFO.: US 2001-998073 A3 20011130

L37 ANSWER 7 OF 35 CAPLUS COPYRIGHT 2005 ACS ON STN
 AB Smog chamber/FTIR techniques were used to study the OH radical and Cl atom initiated oxidation of CF₃OCF₂CF₂ in 700 Torr of air at 296 K. Using relative rate techniques it was determined that $k(\text{OH} + \text{CF}_3\text{OCF}_2\text{CF}_2) = (2.6 \pm 0.3) \times 10^{-12}$ and $k(\text{Cl} + \text{CF}_3\text{OCF}_2\text{CF}_2) = (3.0 \pm 0.4) \times 10^{-11}$ cm³ mol⁻¹ s⁻¹. Cl atoms initiated atmospheric oxidation of CF₃OCF₂CF₂ gives COF₂ and CF₃OC(O)F in molar yields of 100%. OH radicals initiated atmospheric oxidation of CF₃OCF₂CF₂ in 700 Torr of air at 295 K gives COF₂, CF₃OC(O)F, and FC(O)C(O)F in molar yields of 90, 53, and 40%. The results are discussed with respect to the atmospheric degradation mechanism of CF₃OCF₂CF₂ and other ethers.
 ACCESSION NUMBER: 2000:164858 CAPLUS
 DOCUMENT NUMBER: 132:255067
 TITLE: Atmospheric degradation of CF₃OCF₂CF₂: kinetics and mechanism of its reaction with OH radicals and Cl atoms
 AUTHOR(S): Mashino, M.; Kawasaki, M.; Wallington, T. J.; Hurley, M. D.
 CORPORATE SOURCE: Department of Molecular Engineering, Kyoto University, Kyoto, 606-8501, Japan
 SOURCE: Journal of Physical Chemistry A (2000), 104(13), 2925-2930
 CODEN: JPACAF; ISSN: 1089-5639
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 REFERENCE COUNT: 15
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L37 ANSWER 6 OF 35 CAPLUS COPYRIGHT 2005 ACS ON STN
 AB CF₃CF₂C(O)F is a suitable source to generate the title radicals which can recombine to give back the precursor or lead to the formation of C₄F₁₀, CF₂O and CO. The authors performed the photolysis of CF₃CF₂C(O)F pure and in the presence of c-C₆H₁₂ or (FCO)₂ (oxalylfluoride), following the concentration of the different species by FTIR spectroscopy. The rate constant for the reaction CF₃CF₂ + FCO → CF₃CF₂C(O)F was obtained through a simulation using both the authors' exptl. data and bibliog. data available. The value found is $(6.8 \pm 0.8) \times 10^{-12}$ cm³ mol⁻¹ s⁻¹ and it is not substantially different from the rate constant $(4.2 \pm 0.5) \times 10^{-12}$ cm³ mol⁻¹ s⁻¹ obtained for the reaction of CF₃ and FCO radicals. Thus, it was concluded that the length of the carbon chain does not affect the mechanism nor the rate constant value when it is compared with the CF₃ + FCO system.
 ACCESSION NUMBER: 2002:452703 CAPLUS
 DOCUMENT NUMBER: 137:223995
 TITLE: Photochemistry of fluorinated compounds: reaction between FCO and CF₃CF₂ radicals
 AUTHOR(S): Malanca, Fabio E.; Bierbrauer, Karina L.; Chiappero, Malisa S.; Arguello, Gustavo A.
 CORPORATE SOURCE: Departamento de Fisicoquímica, Facultad de Ciencias Químicas, INFIQC, Universidad Nacional de Córdoba, Ciudad Universitaria, Córdoba, 5000, Argent.
 SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (2002), 149(1-3), 9-13
 CODEN: JPPCEJ; ISSN: 1010-6030
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 REFERENCE COUNT: 28
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L37 ANSWER 8 OF 35 CAPLUS COPYRIGHT 2005 ACS ON STN
 AB The photolysis at 254 nm of perfluoroacetyl fluoride (CF₃COF) in the gas phase yields C₂F₆, CF₂O and CO as products. An excess of O₂ added to the system leads to the formation of CF₂O and CO₂ as main products. If, instead of O₂, c-C₆H₁₂ were added, the main products are CF₃H and HC(O)F. In both cases a faster rate of CF₃COF disappearance is observed. The measurement of the quantum yield for CF₃COF consumption as well as for products formation are: for CF₃COF alone, $\phi(\text{CF}_3\text{COF}) = 2\phi(\text{C}_2\text{F}_6) = 2\phi(\text{CF}_2\text{O}) = 0.43 \pm 0.05$; in the presence of c-C₆H₁₂ $\phi(\text{CF}_3\text{COF}) = \phi(\text{CF}_3\text{H}) = 1.02 \pm 0.02$ and in the presence of O₂, $\phi(\text{CF}_3\text{COF}) = 1.02 \pm 0.05$. The low quantum yield observed for pure CF₃COF suggests the occurrence of the recombination reaction: CF₃ + FCO → CF₃COF, for which the authors calculated the rate constant as $(6.9 \pm 0.8) \times 10^{-12}$ cm³ mol⁻¹ s⁻¹.
 ACCESSION NUMBER: 1999:220355 CAPLUS
 DOCUMENT NUMBER: 131:51852
 TITLE: Photochemistry of perfluoroacetyl fluoride. Kinetics of the reaction between CF₃ and FCO radicals
 AUTHOR(S): Bierbrauer, K. L.; Chiappero, M. S.; Malanca, F. E.; Arguello, Gustavo A.
 CORPORATE SOURCE: Facultad de Ciencias Químicas, Departamento de Fisicoquímica, INFIQC, Universidad Nacional de Córdoba, Córdoba, 5000, Argent.
 SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (1999), 122(2), 73-78
 CODEN: JPPCEJ; ISSN: 1010-6030
 PUBLISHER: Elsevier Science S.A.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 REFERENCE COUNT: 20
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L37 ANSWER 9 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Difluorovinylidene is a highly reactive and extremely electrophilic singlet carbene that thermally abstrs. an oxygen atom from CO₂ at temps. as low as 30 K. The resulting difluoroketene is characterized for the first time using IR spectroscopy in combination with isotopic labeling and d. functional theory (DFT) calcns. The three observed IR absorptions of the ketene at 1274, 1427, and 2162 cm⁻¹ are assigned to the asym. FCF stretching vibration and the asym. and sym. CCO stretching vibrations, resp. The oxidation of difluorovinylidene with 3O₂ results in a complex product mixture with CF₂, C₂F₄, CO₂, COF₂, and CO as the major products.

A mechanism consistent with all observed products is proposed.

ACCESSION NUMBER: 1998:624946 CAPLUS
 DOCUMENT NUMBER: 129:275569
 TITLE: Oxidation of difluorovinylidene
 AUTHOR(S): Kotting, Carsten; Sander, Wolfram; Senzlober, Michael;
 CORPORATE SOURCE: Burger, Hans
 SOURCE: Lehrstuhl Organische Chemie II, Ruhr-Universitat, Bochum, D-44780, Germany
 PUBLISHER: Chemistry--A European Journal (1998), 4(9), 1611-1615
 DOCUMENT TYPE: CODEN: CEJUED; ISSN: 0947-6539
 LANGUAGE: Wiley-VCH Verlag GmbH
 REFERENCE COUNT: English
 THIS 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L37 ANSWER 10 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The compds. pip+CF₃O-, pip+CF₃CF₂O-, pip+(CF₃)₂CFO-, and (CH₃)₄N+OCF₂O- (pip+ = 1,1,3,3,5,5-hexamethylpiperidinium) are obtained from pip+F- or (CH₃)₄N+F- and COF₂, CF₃COF, (CF₃)₂CO, and (COF)₂. The structures of pip+CF₃CF₂O-, pip+(CF₃)₂CFO-, and (CH₃)₄N+OCF₂O- have been investigated by single-crystal X-ray crystallog. Crystal data are as follows: for pip+CF₃CF₂O-, monoclinic P2₁/c, a = 1300.7(1) pm, b = 828.0(1) pm, c = 1513.3(2) pm, β = 110.13(1)°, Z = 4; for pip+(CF₃)₂CFO-, monoclinic P2₁/c, a = 1182.2(1) pm, b = 1032.9(2) pm, c = 1459.1(1) pm, β = 107.45(1)°, Z = 4; for (CH₃)₄N+OCF₂O-, tetragonal P₄/h₂nm, a = 1115.9(1) pm, c = 1377.1(1) pm, Z = 8. All anion structures are indicative of a neg. hyperconjugation effect. The structure of FOCF₂O- is clearly nonsym. and resembles a close to planar cis oxygen configuration with one addnl. fluorine bound to one carbon atom. This fluorine atom is positioned slightly toward the second carbon atom, which corresponds to a movement from the asym. to the sym. fluorine-bridged structure. Interionic forces seem to be responsible for this peculiar structure. These findings are compared with structures predicted by ab initio calcns.

ACCESSION NUMBER: 1997:720505 CAPLUS
 DOCUMENT NUMBER: 127:346015
 TITLE: The OCF₂F-, OCF(CF₃)₂-, and OCF₂CF₂O- Anions: Preparation and Structure
 AUTHOR(S): Zhang, X.; Seppelt, K.
 CORPORATE SOURCE: Institut fuer Anorganische und Analytische Chemie, Freie Universitaet, Berlin, 14195, Germany
 SOURCE: Inorganic Chemistry (1997), 36(25), 5689-5693
 PUBLISHER: CODEN: INOCHA; ISSN: 0020-1669
 DOCUMENT TYPE: American Chemical Society
 LANGUAGE: Journal
 REFERENCE COUNT: English
 THIS 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L37 ANSWER 11 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Laser-induced fluorescence spectra of FCO are reported between 29,000 cm⁻¹ and 32,800 cm⁻¹. FCO was prepared by three sep. procedures: photolysis of CF₂O and C₂F₂O₂, and photolysis of F₂ in the presence of CO. The observation of the same spectral features from all three production schemes confirms the assignment of FCO as the spectral carrier. Although the LIF spectrum lies in the same wavelength region as the UV absorption spectrum, the two spectra do not have the same appearance and so represent different upper states. The LIF spectrum is assigned as a transition to the A'' Renner-Teller component of a linear 2Π state predicted by ab initio calcns. The spectrum shows a progression of bands at approx. 430 cm⁻¹ intervals, in good agreement with the predicted spacing of bending levels in the 2Π state. The lower frequency stretching mode ν₁ occurs at approx. 960 cm⁻¹. The vibronic bands are strongly degraded to the red, consistent with the calculated geometry of the linear state but not the bent A' state to which the absorption spectrum in this region is assigned. Resolved emission from the longest wavelength prominent bandhead at 29,872 cm⁻¹ shows progressions in the C-O stretch and bend modes of the ground state. The fluorescence lifetime of this band extrapolated to zero pressure is 95 ± 4 ns, while that of the band at 31,136 cm⁻¹ is 63 ± 5 ns.

ACCESSION NUMBER: 1997:187601 CAPLUS
 DOCUMENT NUMBER: 126:310347
 TITLE: Laser-induced fluorescence spectrum of the FCO radical
 AUTHOR(S): Williams, Bradley A.; Fleming, James W.
 CORPORATE SOURCE: Chemistry Division, Code 6185, Naval Research Laboratory, Washington, DC, 20375-5342, USA
 SOURCE: Journal of Chemical Physics (1997), 106(11), 4376-4382
 PUBLISHER: CODEN: JCPSA6; ISSN: 0021-9606
 DOCUMENT TYPE: American Institute of Physics
 LANGUAGE: English

L37 ANSWER 12 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Steady-state photolysis of oxalylfluoride (FC(O)C(O)F) together with FTIR-spectroscopy has been used to investigate the reactions of FCO and FC(O)OO radicals in the presence of O₂ and NO₂. Formation of FCO radicals has been identified as the main photodissocn. process of oxalylfluoride at λ = 254 nm. However, a quantum yield of ν_{ph} = 0.11 ± 0.02 was attributed to the direct formation of CF₂O and CO in this process.

In the presence of O₂, the products of reactions of FC(O)Ox (x = 0,1,2) radicals were bis-fluoroformylperoxide (FC(O)OOC(O)F) and bis-fluoroformyltrioxide (FC(O)OOOC(O)F), as well as CF₂O, CO and CO₂. Addition of NO₂ to the reaction system led to the formation of fluoroformylperoxynitrate (FC(O)OON₂O). The rate constant for the thermal decomposition of fluoroformylperoxynitrate in the temperature range 275-307 K was measured to be k(T) = 3./5 + 1016 exp (-13900-2600+1700/T) s⁻¹. For bis-fluoroformyltrioxide, a rate constant for thermal decomposition of + 10-4 s⁻¹ was measured at temps. around 250 K. The thermal stability of bis-fluoroformyltrioxide and fluoroformylperoxynitrate is discussed in terms of a comparison with the stability of similar mols.

ACCESSION NUMBER: 1996:257599 CAPLUS
 DOCUMENT NUMBER: 124:356008
 TITLE: FTIR-spectroscopic study of reactions of FCO and FC(O)OO radicals in the presence of O₂ and NO₂
 AUTHOR(S): Bednarek, G.; Arguello, G. A.; Zellner, R.
 CORPORATE SOURCE: Inst. Physikalische Theoretische Chemie, Univ. Essen, Essen, D-45117, Germany
 SOURCE: Berichte der Bunsen-Gesellschaft (1996), 100(4), 445-54
 PUBLISHER: CODEN: BBPAUX; ISSN: 0940-483X
 DOCUMENT TYPE: VCH
 LANGUAGE: English

L37 ANSWER 13 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The polyfluoro aromatic ethers C6F5CH2ORF [RF = CF3, C2F5, CH2CF3, CF(CF3)2, C(CF3)3, C(CF3)2C6F5, C(CF3)2OCH2CF3, C(C6F5)2CF3], 4-CF3CH2OC6F4CH2OCH2CF3, and C6F5CH2OCF2CF2OCH2C6F5 were synthesized from C6F5CH2Br in the presence of CsF by reaction with the perfluoro carbonyl compds. COF2, CF3C(O)F, C6F5COF, (C6F5)2CO, (CF3)2CO, and (COF)2; reaction with polyfluoro siloxanes CF3CH2OSi(CH3)3 and C6F5OSi(CH3)3; or reaction with polyfluoroalkoxides generated from the fluorinated silanes CF3Si(CH3)3, C6F5Si(CH3)3, and CF3CH2OSi(CH3)3 reacting with the carbonyl compds. listed above. Single-crystal X-ray anal. of C6F5CH2OC(C6F5)2CF3 was reported. Reactivities of the carbonyl substrates and the silicon-containing reagents are discussed as a function of the alkyl (aryl) substituents present.

ACCESSION NUMBER: 1995:903124 CAPLUS
 DOCUMENT NUMBER: 124:116744
 TITLE: Synthesis of Polyfluoro Aromatic Ethers: A Facile Route Using Polyfluoroalkoxides Generated from Carbonyl and Trimethylsilyl Compounds
 AUTHOR(S): Nishida, Masakazu; Vij, Ashwani; Kirchmeier, Robert L.; Shreeve, Jean'ne M.
 CORPORATE SOURCE: Department of Chemistry, University of Idaho, Moscow, ID, 83844, USA
 SOURCE: Inorganic Chemistry (1995), 34(24), 6085-92
 CODEN: INOCAJ; ISSN: 0020-1669
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:116744

L37 ANSWER 14 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The laser flash photolysis-absorption technique has been used to study the F+FCO+M+CF2O+M recombination reaction between 20 and 700 Torr of M = CF4 at 296 K. The values $k_{rec,0} = (5.6 \pm 1.2) \times 10^{-29}$ [CF4] cm³ mol⁻¹ s⁻¹ and $k_{rec,\infty} = (7.9 \pm 1.1) \times 10^{-11}$ cm³ mol⁻¹ s⁻¹ were determined by extrapolation of the fall-off curve. An anal. of $k_{rec,0}$ with respect to energy-transfer properties has been carried out. The measured $k_{rec,\infty}$ value is in reasonable agreement with the predictions of the simplified statistical adiabatic channel model. For the FCO+FCO+CF2O+CO reaction a rate coefficient of $(2.1 \pm 0.2) \times 10^{-11}$ cm³ mol⁻¹ s⁻¹ was determined

ACCESSION NUMBER: 1995:627773 CAPLUS
 DOCUMENT NUMBER: 123:127247
 TITLE: Kinetics of the recombination reaction between F atoms and FCO radicals
 AUTHOR(S): Cobos, C. J.; Croce, A. E.; Castellano, E.
 CORPORATE SOURCE: Instituto de Investigaciones Fisicoquimicas Teoricas y Aplicadas (INIIFTA), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, de Correo 16, Sucursal 4, (1900) La Plata, Argent.
 SOURCE: Chemical Physics Letters (1995), 239(4,5,6), 320-5
 CODEN: CHPLBC; ISSN: 0009-2614
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 15 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Acyclic polyfluoro mono and disiloxanes CF3CH2OSiMe3 (1), CF3C(CH3)2OSiMe3 (2), CH3C(CF3)2OSiMe3 (3), C6H5C(CF3)2OSiMe3 (4), (CF3)2CHOSiMe3 (5), (CF3)3COSiMe3 (6), FCH2CH2OSiMe3 (7), HCF2CF2CH2OSiMe3 (8), n-C7F15CH2OSiMe3 (9), (CF2CH2OSiMe3)2 (10), and CF2(CF2CH2OSiMe3)2 (11) are synthesized by the reactions of their resp. alcs. with hexamethyldisilazane. Reactions of 1 with CH2Br2, (CNF)3, CFBBr3, perfluorocyclobutene, and C6F5CN proceed readily in the presence of fluoride ion to form CH2(Rf)2 (12), C6H5C(Rf)3 (13), C(Rf)4 (14), [cyclic] CF2C(Rf):C(Rf)CF2 (15), [cyclic] CF2C(Rf):C(F)CF2 (16) and 4-RfC6F4CN (17) (when reacted 1:1) and (Rf)5C6GN (18) (when reacted with excess of 1), resp. (Rf = OCH2CF3). Reactions of 2 with C6F5CN, C6F6, CF3C6F5, ClC6F5, NC5F5, 1,2-diiodotetrafluorobenzene and perfluorocyclobutene in the presence of fluoride ion gave RfC6F4CN (19) or (Rf)2C6F3CN (20) (depending on the ratio of reactants), RfC6F5 (21), RfC6F4CF3 (22), RfC6F4Cl (23), RfC5F4N (24), RfC6F3I2 (25), and [cyclic] CF2C(Rf):C(F)CF2 (26), resp. (Rf = CF3C(CH3)2O). Reactions of 3 with C6F5CN, C6F6 and 1,2-diiodotetrafluorobenzene with fluoride ion as catalyst form RfC6F4CN (27), RfC6F5 (28) and RfC6F3I2 (29), resp. (Rf = CH3C(CF3)2O). Reactions of 4 with CF3C6F5, C6F5CN, perfluorocyclobutene, C6H5CH2Br and CH3I gave RfC6F4CF3 (30), RfC6F4CN (31), [cyclic] CF2C(Rf):C(F)CF2 (32), RfCH2C6H5 (33) and RfCH3 (34), resp. (Rf = C6H5C(CF3)2O). Reactions of 5 with C6F5CN and CF3C6F5 result in RfC6F4CN (35) and RfC6F4CF3 (36), resp. (Rf = (CF3)2CHO). Siloxanes 6, 7, 8 and 9 with C6F5CN form CnC6F4OC(CF3)3 (37), FCH2CH2OC6F4CN (38), HCF2CF2CH2OC6F4CN (39) and n-C7F15CH2OC6F4CN (40). Disiloxane 10 with CH2Br2, Br2CHCHBr2, SOF2, SO2Cl2, COF2, C6F5CN, (COF)2, C5F5N, CF3SO2F, 1,2-diiodotetrafluorobenzene, I(CF2)2O(CF2)2SO2F, FC(O)(CF2)3C(O)F and 1,4-dibromotetrafluorobenzene gave polyfluorinated cyclic or acyclic ethers [cyclic] CF2CH2OCH2OCH2CF2 (41), [cyclic] CF2CH2OCH2OCH2CF2 (42), [cyclic] CF2CH2OS(O)OCH2CF2 (43), [cyclic] CF2CH2OSO2OCH2CF2 (44), FC(O)OCH2CF2CF2CH2OC(O)F (45), 4-CNC6F4OCH2CF2CF2CH2OC6F4CN-4 (46), [cyclic] CF2CH2OC(O)C(O)OCH2CF2 (47), [cyclic] CF2CH2OP(O)FOCH2CF2 (48), NC5F4OCH2CF2CF2CH2OC5F4N (49), CF3SO2OCH2CF2CF2CH2OSO2CF3 (50), ClOH4F6I2O2 (51), I(CF2)2O(CF2)2SO2OCH2CF2 (52), CF2CH2O(CF2)2I (52), [cyclic] CF2CH2OC(O)(CF2)3C(O)OCH2CF2 (53), and Cl4H8F8Br2O4 (54), resp.

Reactions of 11 with CH2Br2, COF2, SOF2, and SO2Cl2 also give cyclic and acyclic ethers [cyclic] CF2CF2CH2OCH2OCH2CF2 (55), FC(O)OCH2CF2)3CH2OC(O)F (56), [cyclic] CF2CF2CH2OS(O)OCH2CF2 (57), and CF2CF2CH2OSO2OCH2CF2 (58), resp. Ethers 17, 38-40 and CH3CH(CF3)OC6F4CN (59) are also prepared by reacting the corresponding alcs. with pentafluorobenzonitrile in the presence of alkali carbonate as the HF-acceptor. Reaction of C6H5OSiMe3 with C6F5CN yields the polyether (C6H5O)5C6GN (60). When ethers 17, 38-40 and 59 are hydrolyzed in alkaline hydrogen peroxide (30%), the corresponding benzamides CF3CH2OC6F4CONH2 (61), FCH2CH2OC6F4CONH2 (62), HCF2CF2CH2OC6F4CONH2 (63), n-C7F15CH2OC6F4CONH2 (64) and CH3CH(CF3)OC6F4CONH2 (65), resp., are formed.

ACCESSION NUMBER: 1995:169421 CAPLUS
 DOCUMENT NUMBER: 122:31596

L37 ANSWER 15 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 TITLE: Synthesis and Chemistry of Acyclic Mono and Disiloxanes: Useful Precursors to Per- and Polyfluoroethers
 AUTHOR(S): Patel, Nimesh R.; Chen, Jianguo; Zhang, Yuan F.; Kirchmeier, Robert L.; Shreeve, Jean'ne M.
 CORPORATE SOURCE: Department of Chemistry, University of Idaho, Moscow, ID, 83844-2343, USA
 SOURCE: Inorganic Chemistry (1994), 33(24), 5463-70
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 122:31596

L37 ANSWER 16 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Exptl. results are presented of a Fourier transform IR product study at 298 K of the reaction system CFO + O2 at oxygen pressures between 3 and 250 mbar. Pulsed photolysis of oxalyl fluoride (CFO)2 or formyl fluoride (CHFO) at 193 nm was used to produce CFO. As stable products were bisfluoroformyl peroxide, carbonyl fluoride and carbon dioxide. The yields of the peroxide and of CF2O were measured as a function of [O2]/[precursor] and are discussed qual.
 ACCESSION NUMBER: 1994:566764 CAPLUS
 DOCUMENT NUMBER: 121:166764
 TITLE: Fourier transform IR product study of the reaction of CFO radicals with O2 at 298 K
 AUTHOR(S): Ahonkhal, Sam I.; Noelle, Andreas; Behr, Peter; Heydtmann, Horst
 CORPORATE SOURCE: Department of Chemistry, University of Benin, Benin-City, Nigeria
 SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (1994), 80(1-3), 389-92
 CODEN: JPPCEJ; ISSN: 1010-6030
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 17 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Si compound layers are etched with inorg. halide gases (A) containing ≥1 functional groups selected from CO, SO, SO2, nitrosyl, or nitril. Optionally, the etchants contain fluorocarbon compds. (B). Two-step etching process comprising just etching with A and B and over etching A and B of higher A/B ratio than the just etching process is also claimed. Dry etching is carried out at high selectivity without contamination.
 ACCESSION NUMBER: 1994:287533 CAPLUS
 DOCUMENT NUMBER: 120:287533
 TITLE: Dry etching
 INVENTOR(S): Yanagida, Toshiharu
 PATENT ASSIGNEE(S): Sony Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05326460	A2	19931210	JP 1993-17617	19930204
JP 3298205	B2	20020702		
US 5445712	A	19950829	US 1993-29534	19930311
PRIORITY APPLN. INFO.:			JP 1992-67111	A1 19920325
			JP 1992-67112	A1 19920325

L37 ANSWER 18 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Trifluoromethyl and pentafluoromethyl moieties are easily transferred to a variety of fluorinated inorg. and organic sulfur and carbon centers by using (trifluoromethyl)trimethylsilane and (pentafluorophenyl)trimethylsilane in the presence of catalytic amts. of fluoride ion. This method is readily applied to the simple, efficient preparation of known, previously difficult to obtain mols., as well as a number of new perfluoroalkyl and perfluoroaryl sulfanes, sulfoxides, ketones, esters, and alcs. In addition, the first stable oxysulfurane containing more than two sulfur-carbon bonds, Me2CF3SOSiMe3, has been prepared
 ACCESSION NUMBER: 1992:407568 CAPLUS
 DOCUMENT NUMBER: 117:7568
 TITLE: Trifluoromethylation and pentafluorophenylation of sulfur and carbon centers using (trifluoromethyl)- and (pentafluorophenyl)trimethylsilane
 AUTHOR(S): Patel, Nimesh R.; Kirchmeier, Robert L.
 CORPORATE SOURCE: Dep. Chem., Univ. Idaho, Moscow, ID, 83843, USA
 SOURCE: Inorganic Chemistry (1992), 31(12), 2537-40
 CODEN: INOCAD; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 117:7568

L37 ANSWER 19 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB MINDO/3, MNDO, AM1, and PM3 calcns. of mol. vibrational frequencies are reported for 61 mols. All techniques were applied to both well-behaved and badly behaved systems. Overall, MINDO/3 and MNDO were found to contain rather large errors whereas AM1 and PM3 were relatively accurate. Since no technique does well for all mols., the technique used should be chosen based on the mol. vibration of interest. In general, AM1 and PM3 together provide fairly accurate results.
 ACCESSION NUMBER: 1991:642582 CAPLUS
 DOCUMENT NUMBER: 113:242582
 TITLE: Calculations of molecular vibrational frequencies using semiempirical methods
 AUTHOR(S): Coolidge, Michael B.; Marlin, John E.; Stewart, James J. P.
 CORPORATE SOURCE: Frank J. Seiler Res. Lab., U. S. Air Force Acad., CO, 80840, USA
 SOURCE: Journal of Computational Chemistry (1991), 12(8), 948-52
 CODEN: JCCHDD; ISSN: 0192-8651
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 20 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The title reaction of hexafluorocyclobutene (I), 1,2-dichloro-3,3,4,4-tetrafluorocyclobutene, and decafluorocyclohexene (II) at total pressure 13.3 and 16 kPa yield (COX)2 (X = F, Cl) and C2F4, which undergo secondary reactions to give COF2, CO and X2. II oxidation is preceded by retro-Diels-Alder decomposition, affording I and C2F4. Two alternative mechanisms for oxidation of the cyclobutenes are presented, one involving a novel cleavage of intermediate bicyclic dioxetanes. (COF)2 decomposition into COF2 and CO is favored over its oxidation
 ACCESSION NUMBER: 1991:246837 CAPLUS
 DOCUMENT NUMBER: 114:246837
 TITLE: Continuous-wave carbon dioxide laser driven oxidation of some perhalocycloalkenes
 AUTHOR(S): Pola, Josef; Vcelak, Jaroslav; Chvatal, Zdenek
 CORPORATE SOURCE: Inst. Chem. Proc. Fundam., Czech. Acad. Sci., Prague, 165 02, Czech.
 SOURCE: Collection of Czechoslovak Chemical Communications (1991), 56(2), 398-405
 CODEN: CCCCAK; ISSN: 0010-0765
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 21 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The hitherto elusive halocarbonyl cations, XCO+ (X = Cl, Br, I), were prepared in SbF5/SO2ClF solution and characterized by 13C NMR at low temperature. The chlorocarbonyl cation, ClCO+, was prepared by three independent methods, namely, ionization of phosgene or oxalyl chloride in SbF5/SO2ClF, or reaction of Cl2/SbF5/SO2ClF solution with carbon monoxide. The bromo and iodo carbonyl cations were prepared using the reaction of Br2 or I2 in SbF5/SO2ClF with CO. Attempted preparation of the corresponding persistent fluorocarbonyl cation, FCO+, by the ionization of oxalyl fluoride gave carbonyl fluoride and CO. No oxalyl dication was observed although theor. calcns. indicate OCCO2+ to be a min. The 13C NMR chemical shift data on the observed halocarbonyl cations indicate strong stabilization of the pos. charge by the nonbonded electron pair back donation by the halogen atom. Ab initio theor. calcns. were also carried out to rationalize the observed results.
 ACCESSION NUMBER: 1991:206423 CAPLUS
 DOCUMENT NUMBER: 114:206423
 TITLE: Stable carbocations. 280. Halocarbonyl cations
 AUTHOR(S): Prakash, G. K. Surya; Bausch, Joseph W.; Olah, George A.
 CORPORATE SOURCE: Donald P. and Katherine B. Loker Hydrocarbon Res. Inst., Univ. South. California, Los Angeles, CA, 90089-1661, USA
 SOURCE: Journal of the American Chemical Society (1991), 113(8), 3203-5
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 22 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The title compds. were prepared by reaction of hexafluoropropylene oxide (I) with fluorinated ketones and acyl fluoride in a polar organic solvent under substantially anhydrous conditions in the presence of, e.g., KI. Thus, I was added to a mixture of (CF2COF)2 in diglyme containing KI and the mixture stirred 45 min to give 35% FOC(CF2)3OCF(CF3)COF and 49% FOCF(CF3)O(CF2)4OCF(CF3)COF.
 ACCESSION NUMBER: 1989:57123 CAPLUS
 DOCUMENT NUMBER: 110:57123
 TITLE: Preparation of (fluoroalkoxy)carbonyl fluorides
 INVENTOR(S): Flynn, Richard M.
 PATENT ASSIGNEE(S): Minnesota Mining and Manufacturing Co., USA
 SOURCE: Eur. Pat. Appl., 8 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 265052	A1	19880427	EP 1987-307480	19870825
EP 265052	B1	19900228		
R: DE, FR, GB, IT, NL				
US 4749526	A	19880607	US 1986-906816	19860912
CA 1296355	A1	19920225	CA 1987-545509	19870827
AU 8778144	A1	19880317	AU 1987-78144	19870908
AU 601481	B2	19900913		
JP 63077835	A2	19880408	JP 1987-227540	19870910
JP 2525426	B2	19960821		
PRIORITY APPLN. INFO.:			US 1986-906816	A 19860912

OTHER SOURCE(S): CASREACT 110:57123; MARPAT 110:57123

L37 ANSWER 23 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Methods are described for the generation of a number of novel oxyfluoride and fluoride sulfide anions of main-group elements by gas-phase ion-mol. reaction sequences. The energetics of transfer of fluoride from these anions to a variety of Lewis acids were studied by using ion cyclotron resonance techniques. The data obtained are used to generalize periodic trends in fluoride ion binding energies of main-group oxides, fluorides, and oxyfluorides. The data reveal a pronounced tendency for tetrahedral and octahedral anions to exhibit a high degree of stability.
 ACCESSION NUMBER: 1987:649003 CAPLUS
 DOCUMENT NUMBER: 107:249003
 TITLE: Trends in gas-phase fluoride ion affinities of main-group oxyfluorides and fluoride sulfides. Generation and characterization of the fluoride adducts of FAsO, FPO, FPO2, F2SiO, F4SO, FBO, F2SiS, FPS, FAsS, F2S2, and S2O by ion cyclotron resonance addition-elimination reactions
 AUTHOR(S): Larson, J. W.; McMahon, T. B.
 CORPORATE SOURCE: Guelph-Waterloo Cent. Grad. Work Chem., Univ. Waterloo, Waterloo, ON, N2L 3G1, Can.
 SOURCE: Inorganic Chemistry (1987), 26(24), 4018-23
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 24 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Laser-induced fluorescence of FCO (I) was studied in an isothermal flow reactor in the pressure range $0.5 \leq P \leq 112.2$ mbar at room temperature. Excitation spectra were obtained in the range $314.5 \leq \lambda \leq 315.5$ nm with a spectral resolution of $\Delta\lambda = 0.15$ nm. Exciting at $\lambda = 315.06$ nm, an emission spectrum was observed in the range $314.5 \leq \lambda \leq 410$ nm with bands separated by ≈ 630 cm⁻¹. The collision free lifetime of the emitting state was $\tau_0 = 40 \pm 3$ ns. The I radicals were generated in various chemical systems: F + CO or HFCO and O + C₂F₄ or C₂F₃Cl or C₂F₃H. I was also produced in a microwave discharge of C₂F₂/Ar and C₂O₂F₂/Ar mixts. No I radicals were obtained in the IR multiphoton dissociation in C₂F₂/Ar and C₂O₂F₂/Ar mixts.

ACCESSION NUMBER: 1986:98710 CAPLUS
 DOCUMENT NUMBER: 104:98710
 TITLE: Laser-induced fluorescence of the fluorooxomethyl (CFO) radicals in the gas phase
 AUTHOR(S): Dornhoefer, G.; Hack, W.
 CORPORATE SOURCE: Max-Planck-Inst. Stromungsforsch., Goettingen, Fed. Rep. Ger.
 SOURCE: Bericht - Max-Planck-Institut fuer Stromungsforschung (1985), (17), 28 pp.
 CODEN: MPSBBR; ISSN: 0436-1199
 DOCUMENT TYPE: Journal
 LANGUAGE: German

L37 ANSWER 26 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Accurate binding energies of F- and Cl- ions to a wide variety of Lewis acids including oxides, fluorides, oxofluorides, and alkyl derivs. of B, C, Si, P, As, and S were determined with ion cyclotron resonances halide-exchange equilibrium techniques. Magnitudes of Cl- and F- binding energies are discussed in terms of periodic trends, substituent effects, scales of Lewis acid hardness and softness, and empirical correlations. The limited data reveal not strong motivation for definitions of a hard-soft character of Lewis acids and bases in the gas phase. Useful thermochem. data are derived for complex anions which are used to estimate crystal lattice energies for salts of complex Cl and F anions. Implications for new synthetic targets and potential catalytic agents are discussed.

ACCESSION NUMBER: 1985:85235 CAPLUS
 DOCUMENT NUMBER: 102:85235
 TITLE: Fluoride and chloride affinities of main group oxides, fluorides, oxofluorides, and alkyls. Quantitative scales of Lewis acidities from ion cyclotron resonance halide-exchange equilibria
 AUTHOR(S): Larson, J. W.; McMahon, T. B.
 CORPORATE SOURCE: Dep. Chem., Univ. New Brunswick, Fredericton, NB, E3B 6E2, Can.
 SOURCE: Journal of the American Chemical Society (1985), 107(4), 766-73
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 25 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB In stoichiometry-dependent reactions, dimethyl sulfoxide (DMSO) reacts with acyl fluorides, R(CO)F (R = F, CF₃), to yield MeSCH₂F and R(CO)OCH₂F, while MeSCH₂Cl and FC(O)OCH₂Cl are obtained with COClF. Oxalyl difluoride, C₂O₂F₂, reacts with DMSO to give MeSCH₂F and FCH₂OCH₂F.

ACCESSION NUMBER: 1985:614800 CAPLUS
 DOCUMENT NUMBER: 103:214800
 TITLE: On the reactions of dimethyl sulfoxide with acyl fluorides - Pummerer rearrangements and formation of monofluoromethyl esters
 AUTHOR(S): Lange, Horst G.; Shreeve, Jean'ne M.
 CORPORATE SOURCE: Dep. Chem., Univ. Idaho, Moscow, ID, 83843, USA
 SOURCE: Journal of Fluorine Chemistry (1985), 28(2), 219-27
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 103:214800

L37 ANSWER 27 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Articles, especially semiconductor wafers, are selectively chemical treated by means of laser-induced dissociation of gases to form the desired reactive species. The laser wavelength is chosen so that only the desired reaction product is obtained. Thus, for selective etching of a SiO₂ layer on a Si wafer, CF₃I is passed into a chamber containing the wafer and irradiated with a 10-ns to 1-μs pulse from a CO₂ laser at 9.6 μm and 1.2 J/cm². The CF₃I dissociated into I and CF₃, and the CF₃ reacted with the SiO₂ to form SiF₄ and O₂, which were pumped out of the system.

ACCESSION NUMBER: 1981:75605 CAPLUS
 DOCUMENT NUMBER: 94:75605
 TITLE: Device and methods for chemical treatment of articles
 INVENTOR(S): Denison, Dean R.; Hartsough, Larry D.
 PATENT ASSIGNEE(S): Perkin-Elmer Corp., USA
 SOURCE: Ger. Offen., 16 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3013679	A1	19801113	DE 1980-3013679	19800409
US 4260649	A	19810407	US 1979-36828	19790507
CH 644898	A	19840831	CH 1980-2879	19800415
NL 8002566	A	19801111	NL 1980-2566	19800502
FR 2456145	A1	19801205	FR 1980-9966	19800505
FR 2456145	B1	19850322		
GB 2048786	A	19801217	GB 1980-15008	19800506
GB 2048786	B2	19830106		
JP 55149643	A2	19801121	JP 1980-59544	19800507
JP 63001097	B4	19880111		

PRIORITY APPLN. INFO.: US 1979-36828 A 19790507

L37 ANSWER 28 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Tertiary amine trihydrofluorides are stable complexes which are distillable in vacuo. They can be handled without hazard and do not corrode borosilicate glass. They are convenient agents in nucleophilic replacement reactions of Cl or Br by F forming homogeneous reaction mixts. often leading to higher yield under very mild conditions. Examples are given for the preparation of FCH₂COMe, cyanuric fluoride, COF₂, (COF)₂ and SF₄.
 ACCESSION NUMBER: 1980:567511 CAPLUS
 DOCUMENT NUMBER: 93:167511
 TITLE: Tertiary amine tris(hydrofluorides) and their use as fluorinating agents
 AUTHOR(S): Franz, R.
 CORPORATE SOURCE: Hauptlab., Hoechst A.-G., Frankfurt/Main, 6230, Fed. Rep. Ger.
 SOURCE: Journal of Fluorine Chemistry (1980), 15(5), 423-34
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 93:167511

L37 ANSWER 29 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Rate consts. for quenching of oxalyl fluoride (3Au) mols. by selected classes of quenchers were investigated using the technique of laser-induced time-resolved phosphorescence. Various inorg., alkane, halogenated alkane, alkene, halogenated alkene, diene and alkyne quenchers were studied. NO had a much larger quenching rate constant than O₂ (6.8 + 1010 and 1.4 + 108 u mol⁻¹ s⁻¹ resp.). The alkane data are consist with a H atom abstraction mechanism. Both alkene and halogenated alkene rate consts. increase as the triplet energy of the particular quencher decreased. Similar correlations of rate consts. and triplet energy levels were found for the diene and alkyne compds. studied. The phosphorescence emission spectrum was recorded and the 3Au state of oxalyl fluoride lie at 85.6 kcal mol⁻¹. A single progression in the ground state v₁ (C = O sym. stretch) is the dominant feature of the spectrum.
 ACCESSION NUMBER: 1980:434152 CAPLUS
 DOCUMENT NUMBER: 93:34152
 TITLE: Quenching of oxalyl fluoride (3Au) molecules
 AUTHOR(S): Karl, R. R., Jr.; Wampler, F. B.; Oldenberg, R. C.; Rice, W. W.
 CORPORATE SOURCE: Los Alamos Sci. Lab., Univ. California, Los Alamos, NM, 87545, USA
 SOURCE: Journal of Photochemistry (1979), 11(6), 375-84
 CODEN: JPCMAE; ISSN: 0047-2670
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 30 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB By treatment with HF in the presence of MeCN at 10-40°, OCF₂ is prepared from OCCl₂ and oxalyl fluoride from oxalyl chloride. The corresponding Br compds. could be used, but this offers no advantage. Fairly small amts. of MeCN are sufficient, but it is preferable to use a mixture with 30-40 mol% HF. The amount of HF should be equal to or greater than the theor. amount, a molar excess of 50-200 mol % being preferable. In the fluorination of oxalyl chloride, a mixture of HF and oxalyl fluoride is evolved, from which the latter can be separated in a cooling trap. When OCCl₂ is used the reaction is carried out in the presence of Et₃N which combines with the HCl, and reacts with neither the substrate nor the product. Sufficient amine should be present to combine with all the HCl. The product can be obtained in yields >70%. In the preparation of oxalyl fluoride no undesirable OCF₂ is found.
 ACCESSION NUMBER: 1980:149403 CAPLUS
 DOCUMENT NUMBER: 92:149403
 TITLE: Carbonyl difluorides
 INVENTOR(S): Franz, Raimund
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 9 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2823981	A1	19791213	DE 1978-2823981	19780601
EP 5803	A1	19791212	EP 1979-101600	19790524
EP 5803	B1	19810513		
R: DE, FR, GB, IT				
US 4260561	A	19810407	US 1979-43736	19790530
JP 54158396	A2	19791214	JP 1979-66924	19790531
JP 62003087	B4	19870123		
PRIORITY APPLN. INFO.:			DE 1978-2823981	19780601

L37 ANSWER 31 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB Introduction of the S₂ linkage into fluorinated compds. is enhanced by the nucleophilic behavior of CF₃SSH (I) toward fluorinated acid halides. Treatment of CF₃COF, CF₃C(O)SCl, COF₂, FCO(CF₂)₃COF, or FCOCOF with I and KF at -25° gives CF₃C(O)SSCF₃, CF₃C(O)SS₂CF₃ and CF₃C(O)SSCF₃, CF₃SSC(O)F and CF₃SSC(O)SSCF₃, CF₃SSC(O)(CF₂)₃C(O)F and CF₃SSC(O)(CF₂)₃C(O)SSCF₃, and CF₃SSC(O)C(O)F and CF₃SSC(O)C(O)SSCF₃, resp. These mono- and bis(trifluoromethyl)disulfanes are colorless, moderately stable liqs. which are separated only with difficulty from the bis(trifluoromethyl)sulfanes which are formed concomitantly. The mechanism of these reactions are discussed.
 ACCESSION NUMBER: 1977:15991 CAPLUS
 DOCUMENT NUMBER: 86:15991
 TITLE: Trifluoromethyl)disulfane. A reactive nucleophile
 AUTHOR(S): Burton, Craig A.; Shreeve, Jean'ne M.
 CORPORATE SOURCE: Dep. Chem., Univ. Idaho, Moscow, ID, USA
 SOURCE: Journal of the American Chemical Society (1976), 98(21), 6545-7
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L37 ANSWER 32 OF 35 CAPLUS COPYRIGHT 2005 ACS on STN
 AB The electronic structures of aliphatic carbonyls, X2CO3, CH3COX, and (XCO)2 (X = H, F, CN, Me) are examined by the INDO method. Variations in the calculated electron d., the n π^* -excitation energy, the electron affinity, and the ionization potential with α -X substitution are explained qual. in terms of the π -attracting and π -donating character of F, the π -attracting nature of CN and XCO, and the σ , π -donating property of Me. The lowest 3n π^* excitation energies and ionization potentials calculated by the unrestricted Hartree-Fock method agree with the exptl. values. The partitioning of the total energy suggests that the C-O bonds of X2CO compds. in the lowest 3n π^* state and the radical anions derived from them are longer than those of the parent mols., owing to the decrease in the electron-core attraction. The C-C bonds in (XCO)2 compds. are cleaved as easily as the C-X bond on thermal activation and electron impact.
 ACCESSION NUMBER: 1975:408870 CAPLUS
 DOCUMENT NUMBER: 83:8870
 TITLE: Electronic structures of several aliphatic carbonyls. Effects of polar substituents
 AUTHOR(S): Yonezawa, Yoshiro; Fueno, Takayuki
 CORPORATE SOURCE: Fac. Eng. Sci. Osaka Univ., Toyonaka, Japan
 SOURCE: Bulletin of the Chemical Society of Japan (1975), 48(1), 22-5
 CODEN: BCSJAB; ISSN: 0009-2673
 DOCUMENT TYPE: Journal
 LANGUAGE: English

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 GI For diagram(s), see printed CA Issue.
 AB NaF in nonaq. tetramethylene sulfone (I), MeCN (II), or HCONMe2 (III) exchanged halogen readily with acid chlorides, α -chloro ethers, CCl3SCl, CCl2, SeOCl2, phosphorus oxychlorides, phosphorus thiochlorides, and phosphonitric chlorides. The majority of the reactions were carried out at atmospheric pressure in pyrex glass and the product collected in glass traps (solid CO2-Me2CO), the gaseous products distilled at low temperature, and the liquids fractionated through a spinning band column or a 10-in. Vigreux column. NaF in I (II, III) was stirred with slow introduction of the chloro compound (sum of wts. in g. of 2 components numerically equal to volume of medium in ml.) below 100° and heating begun after addition of all reactant. CF3SCl and CF3SSCF3 (3:2 by weight) were obtained in 47% yield by heating NaF with CCl3SCl in I at 170-250°. FCOCN was produced in 14% yield by reaction of COCl2 at room temperature with NaF in HCN. Conditions for the synthesis of carbon fluorides were tabulated [reactants (moles), reaction conditions (temperature/hrs.), % conversion of chloride to fluoride, and products (b.p.) given]: CCl2 (1.03), I (2.18), NaF (2.62), 33-85°/1.0, 89-122°/3.0, 122-224°/0.6, 224-45°/0.2, 37, CF3SSCF3 (31-5°), CS2, CCl3SCl (1.09), I (3.16), NaF (4.76), 34-107°/0.5, 107-209°/1.3, 209-240°/2.75, 47, CF3SCl (-4 to +2°), CF3SSCF3 (27-37°); (NCCl)3 (0.67), I (1.85), NaF (2.50), 43-134°/0.2, 134-93°/0.4, 193-248°/0.2, 74, (NCF)3 (72.5-3.5°); ClCH2OMe (1.29), I (1.33), NaF (1.90), 33-100°/1.5, 100-145°/1.0, 145-168°/0.7, 47, FCH2OMe (8.0-11.5°); CH2O.CHCl.CHClO.CH2 (0.50), I (1.33), NaF (1.50), 32.93°/0.7, 93-143°/1.0, 143-73°/0.75, 42, CH2O.CHF.CHF.O.CH2 (28-30°/21 mm.); ClCO2Me (1.00), I (1.33), NaF (2.00), 33-81°/0.7, 81-119°/1.4, 119-40°/1.5, 33, FCO2Me (35-7°); (COCl)2 (0.50), I (1.33), NaF (2.00), 59-89°/1.5, 89-122°/2.0, 60, (COF)2 (0-2°), COF2; AcCl (1.02), I (1.33), NaF (2.00), 41-60°/1.5, 60-95°/2.4, 48, AcF (19-20.5°); BzCl (1.00), I (1.33), NaF (1.50), 29-128°/0.4, 128-188°/0.5, 188-226°/0.6, 226-250°/0.4, 62, BzF (157.9°); COCl2 (2.00), HCN (2.04), NaF (9.52), 25°/20 hrs. in 1 l. reactor at autogenous pressure, 14, FCOCN (-20 to -18°), COF2; COF2 (1.00), HCN (1.00), AcOH (3 drops), 150°/3 hrs. in 1 l. reactor and product kept 24 hrs. at 25° in evacuated pressure reactor, 22.5, FCOCN (-22 to -19°). In the syntheses of S and Se oxyfluorides, the reaction media I, II and III were apparently interchangeable: SOCl2 (0.50), NaF (2.00), II (2.88), 43-69°/0.4, 69-80°/1.6, 77, SOF2 (-43 to -36°); SOCl2 (0.50), NaF (2.00), I (1.58), 44-70°/0.5, 70-8°/2.0, 52, SOF2 (-39 to -36°); SO2Cl2 (0.50), NaF (2.48), II (3.24), 80°/3.5, 64, SO2FCl (3-7°); SO2Cl2 (0.50), NaF (2.00), III (1.93), 52-80°/1.1, 80°/1.1, 55, 1:2 SO2F2 (-49 to -48°)-SO2ClF (3-6°); SO2Cl2 (1.00), NaF (4.00), I (2.50), 60°/1.0, 80°/1.0, 100-15°/0.5, 28, SeOF (30-2°/6 mm.). NaF in I exchanged F for Cl bonded to P with formation of phosphorus fluorides: POCl3 (0.49), NaF (2.00), I (1.33), 48-80°/0.4, 80-96°/2.8, 96-168°/0.5,

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 AB FCO was obtained in a CO and in an Ar matrix at 4, 14, and 20°K. by the reaction with CO of F atoms produced upon photolysis of OF2, of NF2, or of trans-N2F2, as well as by the photolysis of F2CO or of HFCO. The 3 vibrational fundamentals of the free radical FCO appear at 1855, 1018, and 626 cm⁻¹. Expts. employing I3Cl6O and I2Cl8O confirm the ir identification of FCO. In uv absorption studies on matrix-isolated FCO, an extensive series of bands was observed between 2200 and 3400 Å. The most prominent progression in this system involves bands spaced at approx. 650-cm⁻¹ intervals. It is likely that this progression is associated with the upper-state bending mode of FCO. F2CO and (FCO)2 are also produced in the reaction of F atoms with a CO matrix, and features of their ir spectra are reported. A supplementary observation of the uv absorption spectrum of gaseous F2CO shows a band system between 1800 and 2100 Å., with spacings of .apprx.1700 cm⁻¹. Presumably this system is contributed by the n π^* carbonyl transition. The approx. geometric structure and the nature of the chemical bonds of FCO are discussed, and the mechanisms of formation of this species and of the other observed products are considered. An estimate of the thermodynamic properties of FCO is given.
 ACCESSION NUMBER: 1965:401023 CAPLUS
 DOCUMENT NUMBER: 63:1023
 ORIGINAL REFERENCE NO.: 63:157c-e
 TITLE: Matrix-isolation study of the reaction of F atoms with CO. Infrared and ultraviolet spectra of the free radical FCO
 AUTHOR(S): Milligan, Dolphus E.; Jacox, Marilyn E.; Bass, Arnold M.; Comeford, J. J.; Mann, D. E.
 CORPORATE SOURCE: Natl. Bur. of Stds., Washington, DC
 SOURCE: Journal of Chemical Physics (1965), 42(9), 3187-95
 CODEN: JCPSA6; ISSN: 0021-9606
 DOCUMENT TYPE: Journal
 LANGUAGE: English

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 168-215°/0.5, 215-28°/0.2, 43, POF3 (-44 to -40°); PhPOCl2 (0.50), NaF (1.50), I (1.33), 75-120°/1.8, 65, PhPOF2 (44°/2.5 mm.); PSCL3 (0.50), NaF (2.00), I (1.33), 37-140°/0.6, 140-70°/2.7, 53, PSF3 (-52 to -48°); PhPSCL2 (0.50), NaF (1.50), I (1.33), 25-89°/0.4, 89-107°/1.8, 73, PhPSF2 (47-9°/3 mm.); (PNC12)3, 4, 5, 6 (4.31), NaF (32.14), II (34.39), 80°/20, 54, (PNF2)3 (51-2°, n3D 1.3183, m. 29-31°), (PNF2)4 (89-9.5°, n3D 1.3449, m. 30°); PCL3 (0.73), NaF (2.74), I (1.85), 47-52°/1.0, 52-75°/0.6, 75-109°/2.5, 18, PF3 (sample contained 35 mole-% PF3, 20 mole-% HCl); ClCH2POCl2 (0.50), NaF (2.00), I (1.33), 60-175°/0.6, 175-94°/0.9, 194-230°/0.5, 76, ClCH2POF2 (112-13°, recovered from the mixt. by heating 30-40 min. at 80-100°/2-3 mm.). Previously AsF3, PbF2, ZnF2 or SbF3 were employed to prep. phosphorus fluorides.
 ACCESSION NUMBER: 1961:98893 CAPLUS
 DOCUMENT NUMBER: 55:98893
 ORIGINAL REFERENCE NO.: 55:18551f-1, 18552a-e
 TITLE: Synthesis of fluorides by metathesis with sodium fluoride
 AUTHOR(S): Tullock, C. W.; Coffman, D. D.
 CORPORATE SOURCE: E. I. du Pont de Nemours and Co., Wilmington, DE
 SOURCE: Journal of Organic Chemistry (1960), 25, 2016-19
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

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 AB cf. C. A. 35, 1024.8. The apparatus previously used for the direct fluorination of organic gases has been adapted to the vapor-phase fluorination of volatile organic liquids. Using the gas volume ratios of F:Me₂CO:N of 6:1:18, 4:1:12, 4:1:8, 3:1:6 and 2:1:4, the following fractions were obtained (liquid volume %): I, b. below -105° (mostly CF₄), 20, 10, 15, 5, 5; II, b. -105° to -61°, 20, 10, 15, 10, 5; III, b. -61° to -35°, 10, 10, 5, 5, 5; IV, b. -35° to -15°, 10, 5, 5, 10; V, b. above -15°, 40, 65, 55, 75, 80. II consists of a mixture of CO₂, SiF₄ and COF₂ and showed 3 distillation plateaus, b. -92° (all 3 components), b. -88° (CO₂ + COF₂) and b. -83° (COF₂). III contains F₃CCOF, b. -59°, and possibly O₂F₂. IV consists of hexafluoroacetone, b. -28°, m. -129°; it is soluble in H₂O without decomposition and yields a semicarbazone, m. 153° (decomposition); the monohydrate also m. 153° (decomposition); it gives some evidence of the formation of a hydrate but the aqueous solution is completely volatile at low temps.; dilute alkali causes complete decomposition, with the apparent formation of F₃CCO₂H. V contains FCH₂Ac, b. 78°, and oxalyl fluoride, b. 26°. The results are explained on the basis of a free-radical, non-ionic mechanism.
 ACCESSION NUMBER: 1941:17892 CAPLUS
 DOCUMENT NUMBER: 35:17892
 ORIGINAL REFERENCE NO.: 35:2855f-1
 TITLE: Action of elementary fluorine upon organic compounds.
 X. The vapor-phase fluorination of acetone
 AUTHOR(S): Fukuhara, Nobukazu; Bigelow, Lucius A.
 SOURCE: Journal of the American Chemical Society (1941), 63, 788-91
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

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COST IN U.S. DOLLARS

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